

Supplementary Table 1 Detailed information on all identified compounds and their reference comparisons

Compound	Formula	Metabolites	Theoretical m/z	m/z	Retention time (min)	Ion mode	Mass Error (ppm)
L-Alan							
1	C ₉ H ₁₈ N ₂ O ₃	yl-L-leucine	203.1390	203.1390	2.73	POS	0.00
2	C ₂₀ H ₂₀ O ₇	Tangeretin	373.1274	373.1278	9.62	POS	1.07
3	C ₁₀ H ₁₆ N ₄ O ₃	opihidine	241.1285	241.1290	0.84	POS	2.07
9-Octad							
4	C ₁₈ H ₃₅ NO	ecenamide	326.2679	326.2690	12.53	NEG	3.37
5	C ₂₇ H ₄₆ O	Epicholesterol	369.3498	369.3510	14.12	POS	3.25
6	C ₂₀ H ₃₂ O ₅	15-epilepersinc	375.2128	375.2135	7.90	POS	1.87
7	C ₂₄ H ₃₆ O ₆	caesaldekarkin	432.2363	432.2372	9.94	POS	2.08
8	C ₃₄ H ₄₆ O ₉	cinobufagin-3-hydroxyanuberate	621.3020	621.3027	10.01	POS	1.13
9	C ₆ H ₆ O ₃	5-Hydroxymethyl-2-furoic acid	109.0287	109.0289	2.63	POS	0.92

		rancarb					
		oxaldeh					
		yde					
		3-Hydr					
		oxy-2-					
10		Methyl					
	C6H7N	pyridin	110.060	110.060			
	O	e	6	3	1.05	POS	-2.73
		Isonicot					
11	C6H6N	inamid	123.055	123.055			
	2O	e	5	4	0.95	POS	-0.81
	C6H11	Pipecol	130.086	130.086			
12	NO2	ic acid	3	3	0.70	POS	0.00
		3,4,5-Tr					
		ihydrox					
13	C7H6O	ybenzal	153.018	153.019			
	4	dehyde	8	0	2.75	NEG	1.96
	C9H6O	Umbell	161.023	161.024			
14	3	iferone	6	0	5.11	NEG	2.48
	C7H6O	Gallic	169.013	169.013			
15	5	acid	3	8	1.82	NEG	2.96
	C9H13	D-syne	150.090	150.091			
16	NO2	phrine	5	2	1.06	POS	4.66
		3,4-Dim					
		ethoxy					
17	C9H12	benzyl	151.074	151.075			
	O3	alcohol	9	4	4.69	POS	3.31
	C5H5N	Guanin	152.056	152.056			
18	5O	e	3	5	0.93	POS	1.32
	C7H7N	Methyl	154.049	154.049			
19	O3	5-hydr	9	9	4.29	POS	0.00

		oxypyri					
		dine-2-					
		carboxy					
		late					
		5,7-Dih					
20		ydroxy					
	C9H6O	coumar	177.018	177.018			
	4	in	5	9	4.78	NEG	2.26
		5,7-Dih					
		ydroxy-					
21		4H-1-be					
		nzopyr					
	C9H6O	an-4-on	177.018	177.018			
	4	e	5	9	5.42	NEG	2.26
22	C6H12	L-Gluc	179.055	179.055			
	O6	ose	5	8	0.80	NEG	1.68
		Chelido					
23	C7H4O	nic aci	182.992	182.993			
	6	d	5	0	0.93	NEG	2.73
		3-O-Me					
24	C8H8O	thylgall	183.029	183.029			
	5	ate	1	5	3.86	NEG	2.19
25	C7H13	Stachy	161.128	161.128			
	NO2	drine	2	3	0.70	POS	0.62
		Conifer					
26	C10H1	yl alco	163.074	163.075			
	2O3	hol	9	4	4.93	POS	3.07
27	C8H15		186.112	186.113			
	NO	Tropine	6	1	4.72	NEG	2.69
28	C10H1	Conifer	179.070	179.070			
	OO3	aldehy	1	2	5.58	POS	0.56

		de					
		(2R,3R,					
		4S,5R)-					
		2-Amin					
29		o-3,4,5,					
		6-tetrah					
	C6H13	ydroxy	180.086	180.086			
	NO5	hexanal	1	4	0.73	POS	1.67
	C7H10	Methyl	205.034	205.034			
30	O7	citrate	4	9	2.00	NEG	2.44
	C7H12	Aceglut	189.086	189.086			
31	N2O4	amide	0	5	1.19	POS	2.64
		3S-hydr					
		oxy-do					
32	C12H2	decanoi	215.164	215.164			
	4O3	c acid	3	8	9.96	NEG	2.32
	C12H1	Ligusti	191.106	191.106			
33	4O2	cide	7	7	10.29	POS	0.00
	C12H1	Senkyu	193.122	193.122			
34	6O2	nolide	3	3	9.57	POS	0.00
	C12H1	Neocni	195.138	195.138			
35	8O2	dilide	0	0	10.22	POS	0.00
		Glucoh					
36	C7H14	eptonic	225.060	225.061			
	O8	acid	8	2	0.55	NEG	1.78
		demeth					
37	C14H1	ylsuber	229.086	229.086			
	4O3	osin	2	6	9.25	NEG	1.75
		9-Hydr					
38	C12H8	oxy-4-	231.029	231.029			
	O5	methox	0	4	6.28	NEG	2.16

		ypso					
		en					
39	C11H6	Bergapt	203.033	203.033			
	O4	ol	9	9	6.31	POS	0.00
40	C11H6	Xanthot	203.033	203.033			
	O4	oxol	5	7	5.78	POS	0.99
		Senkyu					
41	C12H1	nolide	205.086	205.086			
	2O3	C	1	0	8.72	POS	-0.49
42	C12H1	Bufoten	205.133	205.133			
	6N2O	in	5	5	2.14	POS	0.00
		2-Penta					
43		noylbe					
	C12H1	nzoic	207.101	207.101			
	4O3	Acid	4	5	7.89	POS	0.48
		Senkyu					
44	C12H1	nolide	207.100	207.101			
	6O4	I	8	5	5.76	POS	3.38
45	C12H8	Methox	217.049	217.049			
	O4	salen	3	4	7.37	POS	0.46
46	C12H8	Bergapt	217.049	217.049			
	O4	en	5	5	7.98	POS	0.00
		N-a-Ac					
47	C8H16	etyl-L-a	217.128	217.129			
	N4O3	rginine	9	2	0.90	POS	1.38
48	C11H1	Fraxidi	223.059	223.059			
	0O5	n	5	8	5.21	POS	1.34
49	C15H1	Chrysi	253.049	253.050			
	0O4	n	4	0	8.83	NEG	2.37
50	C12H1	Senkyu	225.111	225.112			
	6O4	nolide	9	0	5.76	POS	0.44

		H					
51	C15H1 2O4	Liquirit igenin	255.064 9	255.065 6			
		Sinapyl			6.04	NEG	2.74
52	C11H1 4O4	alcoho l	255.086 2	255.086 8			
		beta-D- N-Acet ylmann			5.29	NEG	2.35
53	C8H15 NO6	osamin e	256.058 3	256.058 8			
					0.82	NEG	1.95
54	C14H1 4O3	Osthen ol	231.101 2	231.101 4			
		8,12-EP OXYEU DESM A-4(14), 7(11)-D IEN-8- OL-12- ONE			8.31	POS	0.87
55							
	C15H2 0O3	OL-12- ONE	231.137 0	231.137 8			
		8,12-EP OXYEU DESM A-4(14), 7(11)-D IEN-12- ONE			9.49	POS	3.46
56							
	C15H2 0O2	IEN-12- ONE	233.153 6	233.153 6			
					10.54	POS	0.00
57	C18H1 8O2	Magnol ol	265.122 2	265.122 8			
					10.55	NEG	2.26
58	C16H1	Dalber	267.064	267.065	7.83	NEG	2.62

59	2O4	gin	9	6			
		2'-O-M					
		ethyliso					
	C16H1	liquiriti	269.080	269.081			
	4O4	genin	9	4	6.43	NEG	1.86
60	C15H1	Microm	243.100	243.101			
	6O4	arin F	6	4	7.27	POS	3.29
61		(2R)-5,7					
		-Dihyd					
		roxy-2-					
		(4-hydr					
		oxyphe					
		nyl)-2,3					
		-dihydr					
		o-4H-c					
	C15H1	hromen	271.060	271.060			
	2O5	-4-one	2	7	6.83	NEG	1.84
62	C9H13	Cytara	244.091	244.092			
	N3O5	bine	8	3	0.90	POS	2.05
63	C9H12	Spongo	245.075	245.076			
	N2O6	uridine	8	3	1.25	POS	2.04
64	C15H1		245.117	245.117			
	6O3	Osthol	2	2	10.35	POS	0.00
65	C17H2	[6]-Sho	275.163	275.164			
	4O3	gaol	5	4	10.47	NEG	3.27
66	C13H1	Isopim	247.059	247.059			
	0O5	pinellin	7	9	8.01	POS	0.81
67	C15H2	Alantol	277.143	277.143			
	0O2	actone	1	8	10.65	NEG	2.53
68	C17H1	N-(p-H	282.112	282.113			
	7NO3	ydroxy	3	0	5.75	NEG	2.13

		phenyl)					
		ethyl p					
		-hydro					
		xycinna					
		mide					
69	C16H1	Genkw	283.059	283.060			
	2O5	anin	8	5	8.98	NEG	2.47
70	C16H1	Acaceti	283.060	283.060			
	2O5	n	0	6	8.80	NEG	2.12
		Spaglu					
71	C11H1	mic Ac	285.071	285.072			
	6N2O8	id	7	0	1.34	NEG	1.05
72	C16H1	Helichr	285.075	285.076			
	4O5	ysetin	8	3	7.74	NEG	1.75
73	C16H1	Isosaku	285.075	285.076			
	4O5	ranetin	6	2	8.94	NEG	2.10
		Isoliqui					
74	C15H1	ritigeni	257.080	257.080			
	2O4	n	0	4	7.55	POS	1.56
75	C15H1	Steppo	287.054	287.055			
	2O6	genin	7	4	6.06	NEG	2.44
76	C15H1	(+)-Cat	289.070	289.071			
	4O6	echin	7	2	4.20	NEG	1.73
77	C15H1	Epicate	289.070	289.071			
	4O6	chin	7	2	4.48	NEG	1.73
		Brevifol					
78		incarbo					
	C13H8	xylic a	291.013	291.014			
	O8	cid	4	0	4.27	NEG	2.06
79	C16H1	Formon	269.080	269.080			
	2O4	onetin	2	5	7.84	POS	1.11

80	C16H1	Hispid	299.054	299.055			
	2O6	ulin	7	4	6.86	NEG	2.34
81	C14H6	Ellagic	300.997	300.998			
	O8	acid	6	3	4.90	NEG	2.33
82	C15H1	Baicalei	271.059	271.059			
	0O5	n	5	8	7.35	POS	1.11
83		Isoliqui					
		ritigeni					
		n 2'-me					
84	C16H1	thy eth	271.095	271.096			
	4O4	er	9	2	6.45	POS	1.11
		Naring					
85	C15H1	enin ch	273.075	273.075			
	2O5	alcone	4	6	6.82	POS	0.37
86	C16H2	Huperz	279.142	279.144			
	0N2O	ine B	9	9	3.85	POS	6.81
		N-palm					
87	C18H3	itoyl gl	312.253	312.253			
	5NO3	ycine	0	7	12.32	NEG	2.24
88	C15H1	Isomer	283.093	283.093			
	6O4	azin	1	6	8.34	POS	1.77
89	C16H1	Wogoni	285.075	285.075			
	2O5	n	5	6	8.80	POS	0.35
90	C16H1	Oroxyli	285.075	285.075			
	2O5	n A	1	4	9.11	POS	1.05
		7-Isoqu					
		inolino					
		l, 1,2,3,					
		4-tetrah					
	C17H1	ydro-1-	286.143	286.143			
	9NO3	((4-hyd	4	6	4.24	POS	0.70

		roxyph enyl)m ethyl)-6 -metho xy-, (R) -					
		Sappan					
91	C16H1	chalcon	287.090	287.090			
	4O5	e	4	9	5.47	POS	1.74
92	C15H1	Isookan	289.070	289.070			
	2O6	in	5	6	4.81	POS	0.35
93	C14H1	BERGE	327.070	327.071			
	6O9	NIN	7	4	4.13	NEG	2.14
		Gamma					
		-Gluta					
94		mylphe					
	C14H1	nylalan	295.128	295.128			
	8N2O5	ine	4	6	4.12	POS	0.68
		Vanillic					
		acid 4					
95		-beta-D					
	C14H1	-glucosi	329.086	329.087			
	8O9	de	4	1	3.21	NEG	2.13
		N2-Met					
96	C11H1	hylgua	298.113	298.114			
	5N5O5	nosine	4	0	2.09	POS	2.01
97	C18H1	Stephar	298.142	298.143			
	9NO3	ine	8	3	4.30	POS	1.68
98	C19H2	Aurapt	299.163	299.163			
	2O3	ene	6	9	11.74	POS	1.00
99	C18H3	Sphing	300.288	300.289	9.36	POS	2.00

	7NO2	osine	5	1			
100	C16H1	Diosme	301.070	301.070			
	2O6	tin	5	6	7.06	POS	0.33
101	C16H1	Tectori	301.070	301.070			
	2O6	genin	1	4	6.86	POS	1.00
		Dihydr					
102	C18H1	otanshi	301.082	301.083			
	4O3	none I	9	2	10.26	POS	1.00
	C11H8	Photinu					
103	N2O3S	s lucife	302.985	302.986			
	2	rin	4	1	5.63	POS	2.31
104	C16H1	Hesper	303.085	303.086			
	4O6	etin	7	0	7.14	POS	0.99
		L-Ascor					
		bic aci					
105	C12H1	d 2-glu	337.075	337.076			
	8O11	coside	4	5	0.91	NEG	3.26
106	C15H1	Daphni	339.070	339.071			
	6O9	n	1	1	3.98	NEG	2.95
107	C17H1		309.086	309.086			
	2N2O4	Flazine	4	7	6.33	POS	0.97
108	C17H1	Syringe	345.059	345.060			
	4O8	tin	8	7	7.20	NEG	2.61
109	C18H1	Noriso	314.137	314.138			
	9NO4	boldine	9	3	4.24	POS	1.27
110	C18H1	Moupi	314.137	314.138			
	9NO4	namide	5	1	5.90	POS	1.91
111	C19H2	Armep	314.174	314.174			
	3NO3	avine	7	9	4.55	POS	0.64
112	C19H2	Marmi	315.157	315.158			
	4O5	n	3	5	7.57	POS	3.81

		Semilic					
113	C20H1	oisoflav	351.085	351.086			
	6O6	one B	8	6	9.40	NEG	2.28
	C16H1	Isorha	317.064	317.065			
114	2O7	mnetin	4	0	7.18	POS	1.89
		Chloro					
115	C16H1	genic a	353.086	353.086			
	8O9	cid	0	9	4.19	NEG	2.55
		5-Caffe					
116	C16H1	oylquin	353.086	353.087			
	8O9	ic acid	2	0	3.78	NEG	2.27
		Licoisof					
117	C20H1	lavone	353.101	353.102			
	8O6	A	3	2	9.71	NEG	2.55
		Glycyrr					
118	C20H1	hisoflav	353.101	353.102			
	8O6	one	5	3	9.48	NEG	2.27
		Tripton					
		oterpen					
119		e meth					
	C20H2	yl ethe	318.236	318.239			
	8O2	r	8	8	10.88	POS	9.43
		Cryptot					
120	C19H2	anshino	319.129	319.130			
	0O3	ne	5	0	11.00	POS	1.57
	C20H2	Mataire	357.133	357.133			
121	2O6	sinol	0	7	6.99	NEG	1.96
		Protosa					
122	C16H1	ppanin	327.086	327.085			
	6O6	B	5	2	4.71	POS	-3.97
123	C19H2	BOLDI	328.154	328.154	4.12	POS	-0.30

	1NO4	NE	5	4			
124	C21H18O6	Glycyrol	365.101	365.102	9.89	NEG	2.74
125	C17H14O7	Jaceosidin	331.080	331.080	7.09	POS	1.21
		Toddalolactone					
126	C16H20O6	olactone	331.114	331.114	6.43	POS	1.21
		Feruloyl quinic acid (isomer of 88, 888)					
127	C17H20O9	Isoanthracic acid	367.101	367.102	4.64	NEG	3.00
128	C21H20O6	droicarin	367.117	367.117	8.28	NEG	2.18
		Glycyrol					
129	C21H20O6	oumarin	367.116	367.117	9.19	NEG	2.45
130	C20H18NO4+	Epiberberine	336.121	336.122	5.58	POS	2.38
		Neocryptotanshinone					
131	C19H22O4	ptotanshinone	337.140	337.140	10.33	POS	0.89
		Anisocoumarin H					
132	C19H22O4	oumarin H	337.140	337.140	9.69	POS	0.89
133	C21H24O6	Phillygenin	371.148	371.149	8.15	NEG	2.69
134	C19H18	Skullcandine	373.090	373.091	9.00	NEG	2.68

	8O8	pflavon e II	9	9			
135	C15H1 6O9	Aesculi n	341.086 3	341.086 5			
					3.99	POS	0.59
	[C20H2 4NO4]	Magnof lorine	342.168 6	342.169 3			
136					4.38	POS	2.05
		4',5,7,8- Tetram					
137	C19H1 8O6	ethoxyf lavone	343.116 8	343.117 2			
					8.27	POS	1.17
		Scutella rein 5, 6,7,4'-te trameth					
138	C19H1 8O6	yl ethe r	343.116 6	343.117 1			
					9.04	POS	1.46
139	C18H1 6O7	Nevade nsin	345.096 4	345.096 7			
					8.78	POS	0.58
	[C21H2 0NO4]	13-Met hylberb	350.133 1	350.135 9			
140					6.30	POS	8.00
		alpha-					
141	C21H2 3NO5	Allocry ptopine	352.152 5	352.153 7			
					5.53	POS	3.41
142	C17H2 4O11	Garden oside	385.112 7	385.113 1			
					4.46	NEG	1.04
		(2R,3R, 4S,5S,6					
143	C16H2 8O7	R)-2-[(2 E)-4-hy	355.171 3	355.172 0			
					5.22	POS	1.97

		droxy-					
		3,7-dim					
		ethyloc					
		ta-2,6-d					
		ienoxy]					
		-6-(hyd					
		roxyme					
		thyl)ox					
		ane-3,4,					
		5-triol					
		6-Hydr					
		oxylute					
		olin 6,					
144		7,3',4'-t					
		etramet					
	C19H1	hyl eth	359.111	359.112			
	8O7	er	9	2	9.57	POS	0.84
	C19H1	Garden	359.111	359.112			
145	8O7	in B	8	1	10.46	POS	1.11
		Deacet					
		ylpseu					
146		dolaric					
	C20H2	acid	364.210	364.211			
	6O5	A	1	0	7.59	POS	2.47
	C12H2	Turano	365.104	365.104			
147	2O11	se	0	7	0.83	POS	1.92
		Ferulic					
		acid 4					
148	C16H2	-glucosi	401.106	401.107			
	0O9	de	7	8	4.04	NEG	2.74
149	C21H2	Glicoric	369.132	369.132	8.28	POS	1.35

	0O6	one	3	8			
150	C16H2	Jasmin	369.151	369.151			
	6O8	oside B	5	7	4.16	POS	0.81
151	C20H2	Isosine	373.126	373.127			
	0O7	nsetin	4	3	7.59	POS	2.41
152	C20H2	Sinense	373.127	373.127			
	0O7	tin	0	6	8.29	POS	1.61
		Pseudo					
153	C21H2	laric A	373.163	373.164			
	6O7	cid C	2	2	7.00	POS	2.68
154	C21H2	Notopt	377.134	377.135			
	2O5	erol	8	4	9.88	POS	1.59
155	C21H2	Liquirit	417.117	417.118			
	2O9	in	9	5	4.88	NEG	1.44
156	C24H2	Levistol	381.205	381.205			
	8O4	ide A	0	5	11.57	POS	1.31
157	C22H2	Licoric	383.148	383.148			
	2O6	one	3	6	9.80	POS	0.78
		20a-hy					
158		droxy					
	C27H4	cholest	385.344	385.345			
	6O2	erol	7	9	13.38	POS	3.11
		Demeth					
159	C20H2	ylnobil	389.122	389.122			
	0O8	etin	7	9	10.04	POS	0.51
		3'-Hydr					
160		oxy-5,6,					
		7,8,4'-p					
		entame					
	C20H2	thoxyfl	389.122	389.122			
	0O8	avone	0	5	7.80	POS	1.54

161	C21H2	Curcu	391.114	391.114			
	0O6	min	4	8	9.46	POS	1.02
162	C21H2		431.096	431.097			
	0O10	Vitexin	2	3	4.81	NEG	2.55
163	C19H3	Roseosi	431.189	431.191			
	0O8	de	7	0	4.48	NEG	3.01
164		(R)-5-Hydroxy-2-(4-hydroxyphenyl)-7-(((2S,3R,4S,5S,6R)-3,4,5-trihydroxy-6-(hydroxymethyl)tetrahydro-2H-pyran-2-yl)oxy)chroman-4-one					
	C21H2	oman-4	433.112	433.113			
165	2O10	-one	0	0	5.16	NEG	2.31
	C17H2	Genipo	433.132	433.133			
	4O10	side	3	7	4.42	NEG	3.23
166	C17H2	Syringi	395.130	395.130			
	4O9	n	1	7	4.16	POS	1.52
167	C21H2	(-)-Arct	395.145	395.146			
	4O6	igenin	5	0	7.86	POS	1.27

168		(2S,3S,4S)-4-(4-hydroxy-3-methoxyphenyl)-2,3-bis(hydroxymethyl)-7-methoxy-3,4-dihydro-1H-naphthal					
	C20H2	ene-2,6-	399.140	399.140			
	4O7	diol	4	9	5.01	POS	1.25
169	C21H2	Nobilet	403.137	403.138			
	2O8	in	9	3	9.02	POS	0.99
170	C25H2	Auranti	403.200	403.200			
	6N2O3	amide	2	9	8.61	POS	1.74
		Eleuthe					
171	C17H2	roside	407.094	407.094			
	0O10	B1	7	8	4.51	POS	0.25
		Oleosid					
172		e 11-m					
	C30H4	ethylest	453.335	453.336			
	6O3	er	4	4	13.25	NEG	2.21
		Wogoni					
173		n 7-glu					
	C22H2	curonid	459.091	459.092			
	0O11	e	7	5	6.27	NEG	1.74

		Querci					
174	C21H2	meritri	463.086	463.087			
	0O12	n	4	3	4.96	NEG	1.94
		Hesper					
		etin 7-					
175	C22H2	O-gluc	463.122	463.123			
	4O11	oside	8	7	5.42	NEG	1.94
	C24H3	Schisan	417.226	417.226			
176	2O6	drin A	2	7	11.61	POS	1.20
	C21H2	Natsud	419.132	419.132			
177	2O9	aidain	1	9	9.65	POS	1.91
	C21H2	Isoliqui	419.132	419.133			
178	2O9	ritin	9	3	5.50	POS	0.95
		Dihydr					
		oartemi					
179	C15H2	sinic ac	471.345	471.346			
	4O2	id	9	9	11.01	NEG	2.33
		Deoxyp					
180	C22H2	odophy	421.124	421.125			
	2O7	llotoxin	8	3	9.43	POS	1.19
	C19H1	Mangif	423.091	423.091			
181	8O11	erol	2	7	4.36	POS	1.18
		Norswe					
182	C19H1	rtianoli	423.092	423.092			
	8O11	n	0	1	4.91	POS	0.24
		13-alph					
		a-(21)-E					
183		poxyeu					
	C20H2	rycoma	425.136	425.140			
	4O10	none	2	2	4.37	POS	9.41
184	C23H2	Paeonif	479.153	479.154	4.68	NEG	2.30

	8O11	lorin	7	8			
185	C26H3	Rutaevi	485.179	485.180			
	0O9	n	9	8	8.03	NEG	1.85
186	C30H4	Quillaic	485.325	485.326			
	6O5	acid	2	2	10.45	NEG	2.06
		Chrysi					
187		n 7-glu					
	C21H1	curonid	431.096	431.096			
	8O10	e	5	9	6.07	POS	0.93
188	C22H2		431.132	431.133			
	2O9	Ononin	9	3	5.59	POS	0.93
189	C21H2	Isovitex	433.112	433.112			
	0O10	in	7	8	4.81	POS	0.23
		3,5,6,7,					
		8,3',4'-					
190		Hepta					
		methox					
	C22H2	yflavon	433.148	433.149			
	4O9	e	7	0	9.45	POS	0.69
		A-D-Gl					
191	C21H3	ucopyr	493.228	493.228			
	6O10	anoside	6	8	5.78	NEG	0.41
		Choero					
192	C21H2	spondi	435.127	435.127			
	2O10	n	2	9	5.07	POS	1.61
		Oxypae					
193	C23H2	oniflori	495.148	495.149			
	8O12	n	6	7	4.11	NEG	2.22
194	C30H4	oleanoli	501.356	501.357			
	8O3	c acid	8	7	12.57	NEG	1.80
195	C21H1	Baicalin	447.091	447.091	5.54	POS	0.89

	8O11		4	8			
		Norwo					
		gonin					
196	C21H1	7-glucu	447.091	447.091			
	8O11	ronide	0	6	5.84	POS	1.34
	C24H3	Schisan	450.248	450.248			
197	2O7	drin	2	4	9.45	POS	0.44
	C21H2	Miscant	451.123	451.123			
198	2O11	hoside	7	6	4.81	POS	-0.22
	C30H4	Maslini	517.351	517.352			
199	8O4	c acid	7	6	11.00	NEG	1.74
	C26H3	Obacun	455.203	455.205			
200	0O7	one	8	1	9.66	POS	2.86
		Ursolic					
		acid					
201		(2-alph					
	C30H4	a-hydro	455.350	455.351			
	8O4	xy-)	2	4	7.79	POS	2.64
		Baicalei					
		n 6-me					
		thyl et					
202		her 7-g					
	C22H2	lucuron	461.106	461.107			
	0O11	ide	8	3	6.04	POS	1.08
	C22H2	Isoscop	463.122	463.123			
203	2O11	arin	5	0	4.95	POS	1.08
		Auranti					
204	C27H2	amide	467.192	467.193			
	8N2O4	acetate	9	5	9.84	POS	1.28
	C19H2	Gaulth	469.130	469.131			
205	6O12	erin	9	3	4.47	POS	0.85

206	C18H3	Melezit	539.135	539.137			
	2O16	ose	6	0	0.87	NEG	2.60
207	C21H2	Cistano	471.148	471.149			
	8O13	side F	7	5	4.20	POS	1.70
208	C26H3		471.200	471.200			
	0O8	Linonin	0	7	8.43	POS	1.49
209		Paeonif					
	C23H2	lorin s	543.115	543.116			
210	8O13S	ulfite	4	6	4.14	NEG	2.21
	C15H1	Pinoba	543.128	543.128			
211	2O5	nksin	1	9	6.83	NEG	1.47
		Chrysi					
212		n 6-C-g					
		lucosid					
213		e 8-C-a					
	C26H2	rabinos	547.143	547.144			
214	8O13	ide	7	7	4.88	NEG	1.83
		5,8-Dih					
215		ydroxy-					
		6,-meth					
216		oxyflav					
		one-7-					
217	C22H2	O-gluc	477.102	477.102			
	0O12	uronide	2	5	5.94	POS	0.63
218		Liquirit					
	C26H3	in apio	549.159	549.160			
219	0O13	side	6	5	4.80	NEG	1.64
		alpha-					
220	C18H3	Maltotr	549.164	549.166			
	2O16	iose	8	0	0.82	NEG	2.19
221	C23H2	Albiflor	481.170	481.170	4.59	POS	-0.42

	8O11	in	8	6			
216	C23H2	Lactiflo	485.141	485.141			
	6O10	rin	0	4	5.56	POS	0.82
217	C25H2	Neoma	583.128	583.129			
	8O16	ngiferin	6	5	3.95	NEG	1.54
218	C21H2	Fabiatri	509.125	509.126			
	6O13	n	8	2	4.30	POS	0.79
219	C27H3	Vicenin	593.148	593.150			
	0O15	2	8	0	4.32	NEG	2.02
220	C28H3	Ponciri	593.184	593.186			
	4O14	n	6	1	6.02	NEG	2.53
221	C27H3	Neoeri	595.165	595.166			
	2O15	ocitrin	1	0	4.80	NEG	1.51
222	C18H3	Gentian	522.201	522.202			
	2O16	ose	5	2	0.88	POS	1.34
		Tigloyl					
223	C28H3	gomisi	523.230	523.230			
	6O8	n H	0	1	10.37	POS	0.19
224	C28H3	Spinosi	607.164	607.165			
	2O15	n	5	7	4.70	NEG	1.98
225	C28H3	Neohes	609.180	609.181			
	4O15	peridin	5	5	5.22	NEG	1.64
226	C18H3	1-Kesto	527.156	527.157			
	2O16	se	9	6	0.84	POS	1.33
		Timosa					
227	C33H5	ponin	623.378	623.379			
	4O8	A1	7	4	11.43	NEG	1.12
		Schisan					
228	C28H3	therin	537.209	537.209			
	4O9	B	3	4	10.81	POS	0.19
229	C18H3	Mannin	543.130	543.131	0.84	POS	1.29

	2O16	otriose	8	5			
		Benzoy					
230	C30H3	lpaeoni	629.186	629.186			
	2O12	florin	0	8	6.54	NEG	1.27
		Galloyl					
231	C30H3	paeonif	631.164	631.165			
	2O15	lorin	9	9	4.96	NEG	1.58
		oleanoli					
		c acid					
		3-O-bet					
232		a-D-glu					
		cosidur					
	C36H5	onic ac	631.384	631.384			
	6O9	id	1	6	10.22	NEG	0.79
		Schisan					
233	C28H3	therin	553.183	553.183			
	4O9	C	6	5	10.83	POS	-0.18
		Angelo					
234	C29H3	ylgomi	553.240	553.240			
	8O9	sin Q	8	8	10.54	POS	0.00
		Schisan					
235	C30H3	therin	559.193	559.193			
	2O9	A	6	7	10.76	POS	0.18
	C30H3	Gomisi	559.194	559.193			
236	2O9	n G	0	9	10.53	POS	-0.18
	C26H2	Vicenin	565.155	565.155			
237	8O14	1	2	2	4.51	POS	0.00
		Prosaik					
238	C36H5	ogenin	663.410	663.411			
	8O8	D	6	0	9.32	NEG	0.60
239	C27H3	Narirut	581.185	581.186	5.05	POS	0.69

	2O14	in	7	1			
		Benzoy					
240	C30H3	lalbiflor	585.195	585.196			
	2O12	in	8	2	6.70	POS	0.85
	C27H3	Melosi	595.165	595.165			
241	0O15	de A	6	7	4.62	POS	0.17
	C28H3	Didymi	595.201	595.202			
242	4O14	n	9	0	6.02	POS	0.17
	C27H3	Eriocitr	597.181	597.181			
243	2O15	in	6	5	4.80	POS	-0.17
		Crypto					
		chlorog					
244	C16H1	enic aci	707.181	707.182			
	8O9	d	7	3	4.19	NEG	0.85
	C24H4	Maltote	711.219	711.219			
245	2O21	traose	6	8	0.80	NEG	0.28
	C41H6	Momor	763.426	763.426			
246	4O13	din Ic	2	8	9.82	NEG	0.79
		Methyl					
247	C29H3	hesper	625.211	625.212			
	6O15	idin	5	1	5.60	POS	0.96
		Spinosi					
		n 6'''-					
248	C38H4	(E)-feru	783.212	783.213			
	0O18	late	6	4	5.06	NEG	1.02
		Timosa					
249	C39H6	ponin	785.432	785.432			
	4O13	AIII	7	8	9.99	NEG	0.13
		Glycyrr					
250	C36H5	hetic a	647.378	647.378			
	4O10	cid 3-O	6	8	9.80	POS	0.31

		-beta-D -glucur onide 6'-O-gal					
251	C30H3	loylalbi	655.161	655.162			
	2O15	florin	9	6	4.95	POS	1.07
		Saikosa					
252	C42H6	ponin	809.468	809.469			
	8O12	E	9	1	9.32	NEG	0.25
		Licorice					
253	C42H6	-saponi	821.395	821.396			
	2O16	n H2	9	2	8.40	NEG	0.37
		Saikosa					
254	C42H6	ponin	825.463	825.464			
	8O13	A	8	0	8.50	NEG	0.24
		Saikosa					
255	C42H6	ponin	825.463	825.463			
	8O13	B1	6	9	8.94	NEG	0.36
		Nystos					
256	C24H4	e Trihy	689.210	689.210			
	2O21	drate	0	6	0.89	POS	0.73
		Zingibr					
257	C42H6	oside R	839.440	839.441			
	6O14	1	3	9	9.55	NEG	1.91
258	C19H1	Isoman	843.161	843.161			
	8O11	giferin	1	8	4.33	NEG	0.83
		Bupleu					
259	C42H7	roside	843.473	843.474			
	0O14	XIII	9	3	6.39	NEG	0.47
260	C39H6	Anema	741.442	741.442			
	6O14	rrhenas	2	4	7.85	POS	0.27

261		aponin					
		I					
		Oleanol					
		ic acid-					
		3-O-glu					
		cosyl(1-					
		2)xylyl					
		(1-3)glu					
		cosidur					
	C47H7	onic ac	925.479	925.479			
	4O18	id	6	9	9.19	NEG	0.32
262		Anema					
		rrhenas					
	C39H6	aponin	757.437	757.437			
	4O14	A2	1	0	9.02	POS	-0.13
263		Timosa					
		ponin					
	C45H7	ponin	947.484	947.485			
	4O18	B III	7	2	6.60	NEG	0.53
264		Timosa					
		ponin					
	C45H7	ponin	965.495	965.495			
	6O19	BII	5	9	5.41	NEG	0.41
265		Saikosa					
		ponin					
	C48H7	ponin	971.521	971.521			
	8O17	H	1	6	7.51	NEG	0.51
266		Saikosa					
		ponin I					
	C48H7	Saikosa	971.521	971.521			
	8O17	ponin I	1	6	7.26	NEG	0.51
267		Anema					
		rrhenas					
	C39H6	aponin	779.418	779.418			
	4O14	III	4	6	8.48	POS	0.26
268	C48H8	Saikosa	973.534	973.536	7.36	NEG	1.44

	0O17	ponin	9	3			
		F					
		Buddlej					
269	C48H7	asaponi	987.516	987.516			
	8O18	n IVb	0	5	8.21	NEG	0.51
		Chikus					
270	C48H7	aikosid	987.519	987.518			
	8O18	e II	2	1	6.49	NEG	-1.11
		Saikosa					
271	C42H6	ponin	803.455	803.455			
	8O13	G	6	4	8.96	POS	-0.25
		Saikosa					
272	C42H6	ponin	803.454	803.454			
	8O13	B2	2	7	8.51	POS	0.62
	C52H8	Jujubos	1089.54	1089.54			
273	4O21	ide B	71	79	7.79	NEG	0.73
	C51H8	Protogr	1109.53	1109.53			
274	4O23	acillin	67	76	5.92	NEG	0.90
		GLYCY					
		RRHIZI					
275	C42H6	C ACI	823.410	823.410			
	2O16	D	5	8	7.89	POS	0.36
	C27H3	Naringi	1159.34	1159.34			
276	2O14	n	77	94	5.06	NEG	1.47
		Licorice					
277	C42H6	saponin	839.404	839.405			
	2O17	G2	9	4	7.43	POS	0.71
	C58H9	Jujubos	1251.59	1251.59			
278	4O26	ide A	68	92	7.12	NEG	1.92
	C44H7	6"-O-A	845.465	845.465			
279	0O14	cetylsai	2	5	9.51	POS	0.35

		kosapo					
		nin A					
		1F-Fruc					
		tofuran					
280	C30H5	osylnys	851.264	851.264			
	2O26	tose	9	4	0.86	POS	-0.59
	C30H5	Maltop	867.236	867.237			
281	2O26	entaose	5	2	0.83	POS	0.81
		Officin					
282	C45H7	alisinin	903.494	903.495			
	6O19	I	8	1	5.72	POS	0.33
		Timosa					
283	C45H7	ponin	903.496	903.495			
	4O18	C	6	7	6.59	POS	-1.00
		Macros					
284	C45H7	temono	919.488	919.489			
	6O20	side J	7	5	5.75	POS	0.87
		Saikosa					
285	C48H7	ponin	927.531	927.531			
	8O17	C	8	5	7.26	POS	-0.32
		1,1,1,1-					
286	C36H6	Kestoh	1013.31	1013.31			
	2O31	exaose	97	82	1.02	POS	-1.48
	C4H4O	Maleic	115.003	115.003			
287	4	Acid	1	4	0.96	NEG	2.61
	C4H5N	Cytosin	112.051	112.050			
288	3O	e	1	8	1.19	POS	-2.68
	C4H4N		113.034	113.034			
289	2O2	Uracil	8	7	1.23	POS	-0.88
	C4H7N	Creatin	114.066	114.066			
290	3O	ine	6	4	0.85	POS	-1.75

291	C6H6N 2O	Nicotin amide Isonicot	123.055 5	123.055 4			
					1.20	POS	-0.81
292	C6H5N O2	inic aci d	124.039 3	124.039 3			
					1.16	POS	0.00
293	C4H9N 3O2	Creatin e	132.076 6	132.076 7			
					1.17	POS	0.76
294	C5H4N 4O2	Xanthin e	151.025 2	151.025 7			
					1.25	NEG	3.31
295	C5H5N 5	Adenin e	136.061 4	136.061 6			
					0.90	POS	1.47
296		2,5-Dih ydroxy					
	C7H6O 4	benzoic acid Pyrocat	153.018 7	153.019 0			
					4.22	NEG	1.96
297	C7H6O 4	echuic acid Protoca	153.018 7	153.019 0			
					4.90	NEG	1.96
298	C7H6O 4	techuic acid Diethyl	153.018 7	153.019 0			
					3.40	NEG	1.96
299	C4H11 O4P	phosp hate	153.031 8	153.032 0			
					1.72	NEG	1.31
300	C5H4N 4O	Hypox anthine N-Acet	137.045 4	137.045 6			
					1.34	POS	1.46
301		yl-L-as					
	C6H9N O5	partic acid	156.029 9	156.029 8			
					1.21	NEG	-0.64
302	C6H10	Meglut	161.044	161.045	1.51	NEG	2.48

	O5	ol	7	1			
		p-Hydr					
		oxycinn					
303	C9H8O	amic a	163.039	163.039			
	3	cid	5	8	4.89	NEG	1.84
	C8H6O	Phthali	165.018	165.018			
304	4	c acid	3	8	4.38	NEG	3.03
		4-Hydr					
		oxyphe					
305		nyl-2-p					
	C9H10	ropioni	165.054	165.055			
	O3	c acid	9	3	4.11	NEG	2.42
		(S)-2-H					
		ydroxy-					
306		3-phen					
		ylpropa					
	C9H10	noic ac	165.054	165.055			
	O3	id	7	2	5.02	NEG	3.03
		3,4-Dih					
		ydroxy					
307		benzen					
	C8H8O	eacetic	167.034	167.034			
	4	acid	4	7	3.80	NEG	1.80
	C5H11	L-Meth	150.057	150.058			
308	NO2S	ionine	9	1	1.20	POS	1.33
		N-Acet					
309	C8H15	yl-L-leu	172.097	172.097			
	NO3	cine	3	6	4.80	NEG	1.74
	C6H8O	Isocitric	173.009	173.009			
310	7	acid	4	0	0.96	NEG	-2.31
311	C6H6O	trans-A	173.008	173.009	1.27	NEG	1.16

	6	conitic acid	8	0			
312	C8H14O4	Suberic acid	173.081	173.081			
			1	5	4.90	NEG	2.31
313	C6H13N3O3	L-Citru lline	174.087	174.087			
			2	8	0.79	NEG	3.45
314	C2H5O5P	Phosphonoacet ic acid	174.954	174.955			
			7	8	0.70	NEG	6.29
315	C5H11NO2	5-Aminovaleric acid	156.042	156.042			
			1	1	0.81	POS	0.00
316	C6H9N3O2	L-Histidine	156.076	156.076			
			6	7	0.71	POS	0.64
317	C9H10O4	Hydroxyphenyl lactic acid	181.050	181.050			
			0	3	3.89	NEG	1.66
318	C8H9NO4	4-Pyridine oxalic acid	182.045	182.045			
			3	6	1.63	NEG	1.65
319	C7H10O7	2-Methylcitric acid	187.024	187.024			
			9	6	1.64	NEG	-1.60
320	C9H16O4	Azelaic acid	187.096	187.097			
			7	1	5.45	NEG	2.67
321	C5H11NO3S	L-Methionine sulfoxide	166.052	166.053			
			8	0	0.90	POS	1.20
322	C7H11N	N-Acet	188.055	188.056	1.30	NEG	2.13

	NO5	yl-L-gl utamic acid L-Phen	6	0			
323	C9H11	ylalani	166.085	166.086			
	NO2	ne	9	1	2.25	POS	1.20
324	C9H13	p-Syne	168.101	168.101			
	NO2	phrine	5	7	1.05	POS	1.19
325	C11H8	Norhar	169.075	169.075			
	N2	mane	8	9	4.37	POS	0.59
		Oxoglu					
326	C5H6O	taric ac	191.018	191.019			
	5	id	9	3	0.89	NEG	2.09
327	C6H14	L-Lysin	169.094	169.094			
	N2O2	e	5	6	0.70	POS	0.59
328	C6H8O	Citric	191.018	191.019			
	7	Acid	6	1	1.21	NEG	3.14
329	C7H12	Quinic	191.055	191.055			
	O6	acid	3	7	0.85	NEG	2.09
		1-Meth					
330	C7H11	yl-L-his	170.092	170.092			
	N3O2	tidine	2	3	0.70	POS	0.59
331	C6H12	Gluconi	195.049	195.050			
	O7	c Acid	8	4	0.85	NEG	3.08
332	C6H14	L-Argi	175.118	175.118			
	N4O2	nine	6	8	0.79	POS	1.14
		N-Meth					
333	C11H1	yltrypt	175.123	175.123			
	4N2	amine	2	1	4.16	POS	-0.57
334	C6H12	1,5-Anh	199.036	199.037			
	O5	ydrosor	3	1	0.94	NEG	4.02

		bitol					
335	C10H18O4	Sebacic Acid	201.1126	201.1129	6.08	NEG	1.49
336	C11H12N2O2	L-Tryptophan	203.0820	203.0823	3.76	NEG	1.48
337	C6H13NO5	D-Glucosamine	180.0859	180.0863	0.87	POS	2.22
338	C6H8O5	2-Oxodipic acid	205.0342	205.0348	1.30	NEG	2.93
339	C9H11NO3	L-Tyrosine	182.0806	182.0809	1.25	POS	1.65
340	C11H13NO3	N-Acetyl-L-phenylalanine	206.0815	206.0819	5.03	NEG	1.94
341	C6H10O8	Mucic acid	209.0293	209.0298	0.91	NEG	2.39
342	C9H8O3	Phenylpyruvic acid	209.0447	209.0451	4.84	NEG	1.91
343	C12H22O4	Dodecanedioic acid	211.1338	211.1336	7.62	NEG	-0.95
344	C8H10O4	3,4-Dihydroxyphenyl glycol	188.0915	188.0916	1.16	POS	0.53
345	C8H16N2O3	Glycylleucine	189.1232	189.1233	2.75	POS	0.53

346	C7H16	H-HoA	189.134	189.134			
	N4O2	rg-OH	2	4	0.83	POS	1.06
347		N6,N6, N6-Tri methyl-					
	C9H20	L-lysin	189.159	189.159			
348	N2O2	e	6	7	0.71	POS	0.53
		alpha-					
349	C6H12	D-gluc	215.032	215.032			
	O6	ose	0	4	0.82	NEG	1.86
350		Undeca					
	C11H2	nedioic	215.128	215.128			
351	0O4	acid	1	5	6.87	NEG	1.86
		3-Hydr					
352		oxyseb					
	C10H1	acic aci	217.107	217.107			
353	8O5	d	0	6	5.02	NEG	2.76
		N-Acet					
354		yl-L-me					
	C7H13	thionin	192.069	192.069			
355	NO3S	e	7	3	4.02	POS	-2.08
		O-Succi					
356		nyl-L-h					
	C8H13	omoser	218.065	218.066			
357	NO6	ine	8	4	1.44	NEG	2.75
		(E)-Fer					
358	C10H1	ulic aci	195.065	195.065			
	0O4	d	0	1	5.09	POS	0.51
359		N-Acet					
	C11H1	yl-L-tyr	222.076	222.076			
360	3NO4	osine	4	8	3.98	NEG	1.80

355	C12H2	Trauma	227.128	227.128			
	0O4	tic acid	1	5	7.28	NEG	1.76
356	C6H12	D-Fruct	203.052	203.052			
	O6	ose	2	4	0.81	POS	0.98
357		Isopent					
	C10H1	enylade	204.121	204.122			
	3N5	nine	4	9	4.90	POS	7.35
358		Alpha-					
		D-Gala					
		ctose 1					
359	C6H13	-phosp	241.011	241.011			
	O9P	hate	7	5	0.90	NEG	-0.83
	C13H8	Urolithi	213.054	213.054			
360	O3	n B	2	4	7.57	POS	0.94
	C9H12		243.060	243.061			
361	N2O6	Uridine	7	5	1.27	NEG	3.29
		2-Hydr					
		oxymyr					
362	C14H2	istic aci	243.195	243.196			
	8O3	d	4	0	11.34	NEG	2.47
363	C10H1	Prolyl-	215.138	215.138			
	8N2O3	Valine	4	7	1.47	POS	1.39
364		Gamma					
		-Gluta					
	C8H14	mylala	219.096	219.097			
365	N2O5	nine	7	1	1.20	POS	1.83
	C9H18	Serylle	219.133	219.133			
	N2O4	ucine	7	8	2.43	POS	0.46
366		D-Pant					
	C9H17	othenic	220.117	220.117			
	NO5	acid	4	7	2.93	POS	1.36

		N-lacto					
366	C12H1	yl-Tyro	252.086	252.087			
	5NO5	sine	6	2	4.17	NEG	2.38
367	C16H3	Palmiti	255.231	255.232			
	2O2	c acid	8	4	13.62	NEG	2.35
		5-Meth					
368	C10H1	yluridi	257.076	257.077			
	4N2O6	ne	9	4	1.75	NEG	1.94
		O-Des					
369		methyl					
	C15H1	angolen	257.081	257.081			
	4O4	sin	1	5	7.64	NEG	1.56
		Glucos					
370	C6H13	e 6-ph	259.021	259.021			
	O9P	osphate	1	7	0.93	NEG	2.70
		gamma					
371		-Gluta					
	C11H2	mylleu	259.128	259.129			
	0N2O5	cine	7	3	3.91	NEG	2.32
		Isoleuc					
372	C11H2	yl-Vali	231.170	231.170			
	2N2O3	ne	1	2	3.87	POS	0.43
		Threon					
373	C10H2	ylisoleu	233.149	233.149			
	0N2O4	cine	4	5	2.78	POS	0.43
374	C10H1		267.072	267.072			
	2N4O5	Inosine	1	8	1.46	NEG	2.62
		N-Lact					
375		oylphe					
	C12H1	nylalan	238.106	238.107			
	5NO4	ine	8	1	5.11	POS	1.26

		2S-hydr					
		oxypal					
376	C16H3	mitic a	271.226	271.227			
	2O3	cid	7	3	12.42	NEG	2.21
	C9H13	Cytidin	244.091	244.092			
377	N3O5	e	6	2	1.17	POS	2.46
		Aspara					
378	C10H1	ginyliso	246.144	246.144			
	9N3O4	leucine	4	6	2.49	POS	0.81
		Aspart					
379	C10H1	yl-Isole	247.128	247.128			
	8N2O5	ucine	6	7	3.04	POS	0.40
		Valylgl					
380	C10H1	utamic	247.128	247.128			
	8N2O5	acid	2	5	1.24	POS	1.21
		Aspart					
381	C10H1	yl-Leuc	247.129	247.128			
	8N2O5	ine	0	9	3.49	POS	-0.40
		alpha-L					
382	C18H3	inolenic	277.215	277.216			
	0O2	acid	9	6	12.40	NEG	2.53
	C9H12	Pseudo	279.037	279.038			
383	N2O6	uridine	3	1	0.85	NEG	2.87
	C18H3	Oleic a	281.247	281.247			
384	4O2	cid	0	8	13.80	NEG	2.84
	C10H1	Guanos	282.082	282.083			
385	3N5O5	ine	7	6	1.45	NEG	2.84
		2'-Deox					
386	C10H1	yadenosine	252.108	252.108			
	3N5O3	sine	7	9	1.37	POS	0.79
387	C10H1	Xantho	283.067	283.067	1.82	NEG	2.47

	2N4O6	sine	0	7			
		Hexade					
388	C16H3	canedio	285.205	285.206			
	0O4	ic acid	9	5	10.37	NEG	2.10
389	C16H3	Palmita	256.262	256.263			
	3NO	mide	9	2	12.65	POS	1.17
		5-Meth					
390	C10H1	ylcytidi	258.107	258.107			
	5N3O5	ne	3	9	1.19	POS	2.32
		N-Acet					
		yl-b-glu					
391		cosami					
	C8H16	nylami	259.073	259.071			
	N2O5	ne	1	1	0.73	POS	-7.72
		Sedohe					
392		ptulose					
	C7H15	7-phos	289.030	289.031			
	O10P	phate	8	9	0.92	NEG	3.81
393	C12H2	Lysylle	260.196	260.196			
	5N3O3	ucine	1	5	1.22	POS	1.54
		Glutam					
394	C11H2	ylisoleu	261.143	261.144			
	0N2O5	cine	9	2	3.02	POS	1.15
395	C18H3	Linoleic	263.235	263.236			
	2O2	acid	7	6	12.12	POS	3.42
		Ricinol					
396	C18H3	eic aci	297.241	297.242			
	4O3	d	9	7	11.16	NEG	2.69
397	C10H1	Adenos	268.102	268.103			
	3N5O4	ine	8	4	1.28	POS	2.24
398	C11H2	Prolyl-	272.170	272.171	1.82	POS	2.20

	1N5O3	Arginine	5	1			
		Arachidonic acid					
399	C20H32O2	Uridine 5'-monophosphate	303.231	303.232			
			5	2	12.85	NEG	2.31
400	C9H13N2O9P	gamma-Glutamylglutamic acid	305.016	305.017			
			9	2	1.13	NEG	0.98
401	C10H16N2O7	Gondolic acid	277.101	277.102			
			6	3	0.94	POS	2.53
402	C20H38O2	Aspartylphenylalanine	309.278	309.279			
			3	1	14.87	NEG	2.59
403	C13H16N2O5	N6-Methyladenosine	281.112	281.112			
			4	8	3.97	POS	1.42
404	C11H15N5O4	2'-O-Methyladenosine	282.118	282.119			
			9	3	2.18	POS	1.42
405	C11H15N5O4	12,13-Dihydroxyoleic acid	282.119	282.119			
			3	5	1.90	POS	0.71
406	C18H34O4	Octadecanoic acid	313.237	313.237			
			0	7	10.01	NEG	2.23
407	C18H34O2	Octadecanoic acid	313.237	313.237	11.12	NEG	1.92

	4O4	canedio	1	8			
		ic acid					
408	C18H3	Oleami	282.278	282.278			
	5NO	de	5	8	12.88	POS	1.06
		Pelargo					
409	C9H18	nic aci	315.252	315.253			
	O2	d	3	2	10.46	NEG	2.85
410	C18H3	Steara	284.293	284.294			
	7NO	mide	8	3	13.88	POS	1.76
		Ophtha					
411	C11H1	Imic ac	290.132	290.133			
	9N3O6	id	9	8	1.21	POS	3.10
		N-(1-D					
		eoxy-1-					
412		fructos					
	C12H2	yl)leuci	294.153	294.154			
	3NO7	ne	5	1	1.45	POS	2.04
		Docosa					
413		hexaen					
	C22H3	oic aci	327.231	327.232			
	2O2	d	4	1	12.64	NEG	2.44
		9E,11Z,					
		13E-oct					
414		adecatr					
	C18H3	ienoic	296.257	296.257			
	0O2	acid	4	9	10.88	POS	1.69
		5'-Meth					
415	C11H1	ylthioa					
	5N5O3	denosin	298.095	298.096			
	S	e	6	2	3.79	POS	2.01
416	C18H3	Palmito	300.288	300.289	12.19	POS	1.67

	7NO2	ylethan	7	2			
		olamid					
		e					
		N-Oleo					
417	C20H3	yl glyci	338.266	338.268			
	7NO3	ne	7	4	12.55	NEG	5.03
		Fructos					
		e 1,6-bi					
418	C6H14	sphosp	338.986	338.987			
	O12P2	hate	6	7	0.97	NEG	3.24
		N2,N2-					
		Dimeth					
419	C12H1	ylguan	312.128	312.129			
	7N5O5	osine	8	5	3.35	POS	2.24
		Dehydr					
		ophyto					
420	C18H3	sphing	316.283	316.284			
	7NO3	osine	4	0	9.75	POS	1.90
		Anand					
		amide					
421	C20H3	(18:2, n	324.288	324.289			
	7NO2	-6)	9	3	11.73	POS	1.23
	C6H12	Scyllo-I	359.117	359.118			
422	O6	nositol	7	6	0.79	NEG	2.51
	C12H2		325.110	325.112			
423	2O11	Sucrose	9	2	1.05	POS	4.00
		Oleoyl					
424	C20H3	thanola	326.304	326.304			
	9NO2	mide	4	9	12.45	POS	1.53
	C15H2	N-(1-D	328.137	328.138			
425	1NO7	eoxy-1-	7	4	2.35	POS	2.13

		fructos					
		yl)phen					
		ylalani					
		ne					
	C10H1	5'-Guan					
426	4N5O8	ylic aci	362.048	362.049			
	P	d	5	6	0.94	NEG	3.04
		Stearoy					
427	C20H4	lethano	328.319	328.320			
	1NO2	lamide	8	4	13.40	POS	1.83
		Adenos					
		ine 2',3'					
428	C10H1	-cyclic					
	2N5O6	phosph	330.056	330.058			
	P	ate	4	1	1.14	POS	5.15
429	C16H1	Oglufa	334.139	334.139			
	9N3O5	nide	1	4	4.37	POS	0.90
		Sedohe					
		ptulose					
430		1,7-bis					
	C7H16	phosph	368.996	368.998			
	O13P2	ate	7	0	0.98	NEG	3.52
		13-Doc					
431	C22H4	osenam	338.341	338.341			
	3NO	ide	3	5	15.16	POS	0.59
		6-(alph					
		a-D-Gl					
		ucosam					
432		inyl)-1					
	C12H2	D-myo-	342.137	342.138			
	3NO10	inositol	9	7	1.07	POS	2.34

433		N-(1-Deoxy-1-fructosyl)tyrosine	344.1326	344.1333	1.23	POS	2.03
434		N-Palmityl Serine	344.2785	344.2790	11.88	POS	1.45
435		Adenosine 5'-monophosphate	348.0674	348.0689	0.93	POS	4.31
436		N-oleoyl L-serine	370.2938	370.2945	12.15	POS	1.89
437		Riboflavin	377.1446	377.1451	4.42	POS	1.33
438		alpha-1-actose	381.0778	381.0786	0.81	POS	2.10
439		Succinyladenosine	384.1134	384.1142	3.35	POS	2.08
440		Adenosine-5'-diphosphate	426.0197	426.0209	1.13	NEG	2.82
441		SAH	429.1277	429.1237	1.33	NEG	-9.09
442		N-Stearoyl	406.3277	406.3287	13.67	POS	1.97

	5NO3	oyl Val	6	4			
		ine					
		N-Oleo					
443	C23H4	yl Glut	411.320	411.321			
	2N2O4	amine	7	2	11.69	POS	1.22
		Flavin					
444	C17H2	monon					
	1N4O9	ucleoti	439.100	439.101			
	P	de	1	0	4.08	POS	2.05
445	C30H4	Betulini	439.356	439.356			
	8O3	c acid	0	8	12.57	POS	1.82
		D-(+)-T					
446	C12H2	rehalos	683.222	683.223			
	2O11	e	6	9	0.86	NEG	1.90
447	C24H4	Stachyo	701.189	701.190			
	2O21	se	3	3	0.89	NEG	1.43
	C20H3	Glutath					
448	2N6O1	ione ox	613.158	613.158			
	2S2	idized	0	6	1.20	POS	0.98
		L-Azeti					
449		dine-2-					
	C4H7N	carboxy	102.055	102.055			
	O2	lic acid	6	3	0.87	POS	-2.94
450	C4H8N	Glycylg	113.035	113.035			
	2O3	lycine	7	4	0.78	NEG	-2.65
		Iminod					
451	C4H7N	iacetic	114.019	114.019			
	O4	acid	7	4	0.89	NEG	-2.63
		3-Hydr					
452	C5H5N	oxypyri	113.071	113.071			
	O	dine	5	2	0.89	POS	-2.65

453	C6H12	D-Leuci	131.070	131.071			
	O3	c acid	6	0	4.72	NEG	3.05
454		3-Hydr					
		oxy-4-a					
	C5H6N	minopy	128.082	128.081			
	2O	ridine	0	9	0.96	POS	-0.78
455	C6H8O	(±)-Fur	129.055	129.054			
	3	aneol	0	8	3.81	POS	-1.55
456		6-amin					
		o-hexa					
	C6H13	noic ac	132.101	132.101			
	NO2	id	9	9	0.90	POS	0.00
457	C6H14	d-Fucit	147.065	147.065			
	O5	ol	1	4	0.80	NEG	2.04
458		2-Hydr					
	C9H10	oxycha	149.060	149.060			
	O2	vicol	0	4	6.43	NEG	2.68
459	C8H11	Vanillyl	136.074	136.075			
	NO2	amine	7	5	0.91	POS	5.88
460		Hydrox					
	C8H10	ytyroso	153.055	153.055			
	O3	l	1	4	3.52	NEG	1.96
461		4'-Hydr					
		oxyacet					
	C8H8O	opheno	137.059	137.059			
	2	ne	9	8	4.96	POS	-0.73
462	C7H7N	Trigone	138.054	138.054			
	O2	lline	7	8	0.89	POS	0.72
463		2-hydro					
	C8H16	xy capr	159.101	159.102			
	O3	ylic aci	7	2	6.66	NEG	3.14

		d					
464	C7H11	Arecaid	142.086	142.086			
	NO2	ine	3	3	0.88	POS	0.00
		Dihydr					
465	C11H1	oactini	161.097	161.096			
	6O2	diolide	0	8	8.16	NEG	-1.24
		1-Deox					
466	C6H13	ynojiri	146.080	146.081			
	NO4	mycin	2	0	0.87	POS	5.48
		N-Meth					
467	C6H11	yl-L-pr	147.112	147.112			
	NO2	oline	4	6	0.84	POS	1.36
468	C6H13	Fagomi	148.096	148.096			
	NO3	ne	4	6	0.89	POS	1.35
		4-Hydr					
469	C6H13	oxyisol	148.097	148.096			
	NO3	eucine	0	9	1.14	POS	-0.68
470	C7H8O		169.049	169.050			
	2	Orcinol	8	2	4.74	NEG	2.37
		D-threo					
471	C4H8O	nic aci	171.005	171.006			
	5	d	6	1	0.94	NEG	2.92
		3-Hydr					
472		oxy-4-					
		methox					
		y-benza					
	C8H8O	ldehyd	153.054	153.054			
	3	e	6	6	5.01	POS	0.00
		Galactu					
473	C6H10	ronic a	175.023	175.024			
	O7	cid	9	1	0.96	NEG	1.14

		3-Amin					
474	C7H7N	osalicyl	154.049	154.049			
	O3	ic acid	7	8	1.49	POS	0.65
		Tyrosin					
475	C10H1	e meth	176.071	176.071			
	3NO3	ylester	4	3	2.86	NEG	-0.57
		7,8-Dih					
476	C9H6O	ydroxy	177.018	177.018			
	4	in	5	9	4.56	NEG	2.26
		2,6-Dim					
477	C11H1	ethylqu	158.096	158.096			
	1N	inoline	0	2	4.36	POS	1.27
		DL-m-					
478	C9H11	Tyrosin	180.065	180.066			
	NO3	e	6	1	1.30	NEG	2.78
		Amino					
479	C8H17	valeric	160.132	160.132			
	NO2	acid be	6	9	0.90	POS	1.87
		taine					
		S-Allyl-					
480	C6H11	L-cystei	162.057	162.058			
	NO2S	ne	9	1	1.69	POS	1.23
481	C10H1	Anabas	163.122	163.122			
	4N2	ine	6	8	1.22	POS	1.23
482	C4H4N	8-Azag	187.012	187.013			
	6O	uanine	9	5	1.46	NEG	3.21
483	C6H8O	Garcini	189.003	189.003			
	8	a acid	9	7	0.94	NEG	-1.06
484	C6H11	N-Hyd	190.071	190.071			
	NO3	roxypip	3	7	1.48	NEG	2.10

		ecolic a					
		cid					
485	C8H8O	Isovanil	169.049	169.049			
	4	lic acid	7	6	4.47	POS	-0.59
		2,2-dim					
486		ethyl-s					
	C6H10	uccinic	191.055	191.055			
	O4	acid	3	7	4.17	NEG	2.09
		2,3,4-Tr					
487		ihydrox					
	C7H6O	ybenzoi	171.028	171.028			
	5	c acid	6	7	3.53	POS	0.58
488	C11H1	Zingero	193.086	193.086			
	4O3	ne	2	6	5.94	NEG	2.07
		(1S,2R,4					
489		S)-(-)-B					
	C12H2	ornyl a	195.138	195.138			
	0O2	cetate	1	6	9.74	NEG	2.56
490	C5H12	L-Arabi	197.065	197.066			
	O5	nitol	5	1	0.83	NEG	3.04
491	C9H6O	Aescule	179.033	179.033			
	4	tin	5	7	4.31	POS	1.12
		4-(3,4-D					
492		ihydrox					
		ypheny					
		l)but-3-					
	C10H1	en-2-on	179.069	179.070			
	0O3	e	8	1	5.27	POS	1.12
493	C10H1	Fusaric	180.101	180.101			
	3NO2	acid	5	7	5.12	POS	1.11
494	C12H1	Harma	183.092	183.091	4.54	POS	-1.09

	0N2	n	1	9			
495	C11H6	Psorale	187.039	187.039			
	O3	n	0	0	7.12	POS	0.00
		Castan					
496	C8H15	osperm	190.106	190.107			
	NO4	ine	8	1	0.87	POS	1.58
		(S)-3-B					
		utyl-1(3					
497		H)-isob					
	C12H1	enzofur	191.106	191.106			
	4O2	anone	9	8	9.71	POS	-0.52
498	C10H8	Scopole	193.049	193.049			
	O4	tin	5	5	5.15	POS	0.00
499	C5H7C	Acivici	196.048	196.048			
	lN2O3	n	3	3	0.76	POS	0.00
500	C6H10	Gulono	223.044	223.045			
	O6	lactone	9	4	0.89	NEG	2.24
		Methyl					
501	C11H1	isoeug	223.096	223.097			
	4O2	enol	8	2	6.43	NEG	1.79
502	C6H14		227.076	227.076			
	O6	Allitol	4	8	0.77	NEG	1.76
503	C12H9	Dictam	200.070	200.070			
	NO2	nine	6	6	8.02	POS	0.00
		Alanyl					
504	C8H15	glutami	200.101	200.102			
	N3O4	ne	6	6	0.95	POS	5.00
505	C15H1	Kaunio	229.122	229.122			
	8O2	lide	4	9	11.26	NEG	2.18
506	C6H13	Deoxy	202.047	202.047			
	NO4	mannoj	8	7	0.76	POS	-0.49

		irimycin					
		n					
507	C15H2	Cupare	203.179	203.179			
	2	ne	2	3	13.39	POS	0.49
508	C15H2	Farneso	205.194	205.195			
	6O	l	3	0	11.49	POS	3.41
509	C11H1	Scopar	207.065	207.065			
	0O4	one	6	4	5.93	POS	-0.97
		Obtuca					
510		rbamic					
	C11H1	acid	237.086	237.087			
	4N2O4	A	7	4	5.92	NEG	2.95
		2'-O-M					
511	C10H1	ethyluri	239.067	239.066			
	4N2O6	dine	0	9	1.89	NEG	-0.42
		Nitrilot					
512	C6H9N	riacetic	209.077	209.077			
	O6	acid	2	0	0.66	POS	-0.96
513	C7H14	Sequoy	239.076	239.076			
	O6	itol	6	9	0.80	NEG	1.25
514	C12H2	Leucyll	243.170	243.170			
	4N2O3	eucine	4	9	4.25	NEG	2.06
		1-Meth					
515		yl-L-try					
	C12H1	ptopha	219.113	219.112			
	4N2O2	n	0	9	4.45	POS	-0.46
516	C13H1	Harmal	232.144	232.144			
	4N2O	ine	6	5	4.57	POS	-0.43
		Manno					
517	C7H14	heptulo	233.062	233.062			
	O7	se	2	7	0.90	POS	2.15

518	C10H1	Vidara	266.087	266.088	1.32	NEG	3.76
	3N5O4	bine	5	5			
519	C13H1	Gastro	267.085	267.086	1.46	NEG	2.62
	8O7	din	5	2			
520	C16H1	Ftaxilid	268.096	268.097	7.14	NEG	2.24
	5NO3	e	7	3			
521	C15H1	Norwo	269.044	269.045	7.16	NEG	1.49
	0O5	gonin	7	1			
522	C13H2	Vomifo	242.174	242.174	5.22	POS	1.24
	0O3	liol	5	8			
523	C16H1	Loureir	271.094	271.096	6.80	NEG	5.16
	6O4	in C	8	2			
524	C13H1	Pimpin	247.060	247.060	8.21	POS	-0.81
	0O5	ellidine	5	3			
525	C14H1	Peuced	247.095	247.096	5.17	POS	3.24
	6O5	anol	5	3			
526		Dihydr			5.74	POS	0.81
	C14H1	oresver	248.127	248.127			
527	4O3	atrol	7	9	2.15	POS	0.00
	C15H2	Alloma	249.196	249.196			
528	4N2O	trine	1	1	4.45	NEG	-5.34
		Boc-D-					
529	C10H1	Glutam	281.094	281.092	7.75	NEG	0.35
	8N2O5	ine	0	5			
530		7-O-me			6.92	NEG	2.46
	C16H1	thyerio	283.060	283.060			
531	4O6	dictyol	5	5	4.87	POS	2.33
	C16H1	Arbori	285.078	285.079			
531	4N2O	ne	6	3	257.080		
	C15H1	Epiafze	257.080	257.080			
531	4O5	lechin	3	8	2.33		

532		3-Methoxy-4',5'-dihydroxy-trans-stilbene					
	C15H14O3	ns-stilbene	287.091	287.091			
			3	9	7.55	NEG	2.09
533	C14H13NO7	Narciclasine	288.051	288.050			
			0	9	4.86	NEG	-0.35
534	C16H28O	Ambroxide	259.207	259.205			
			8	5	12.83	POS	-8.87
535		Indole-3-methanamine					
	C9H10N2	anamine	291.157	291.159			
			4	4	10.62	NEG	7.21
536		L-beta-aspartyl-L-aspartic acid					
	C8H12N2O7	artic acid	293.061	293.062			
			3	0	0.78	NEG	2.39
537	C16H10N2O2	Indigotin	263.080	263.081			
			7	1	6.33	POS	1.52
538		Norwogonin					
		5,7,8-trimethyl ether					
	C18H16O5	methyl ether	293.085	293.083			
			2	3	8.01	NEG	-6.48
539	C11H20O6	Crenulatin	293.122	293.123			
			8	5	4.20	NEG	2.39
540	C15H28O2	Exaltolide	263.202	263.200			
			0	1	10.24	POS	-7.22
541	C18H18	Danshen	295.102	295.100	9.91	NEG	-8.47

	6O4	nxinku	6	1			
		n A					
542	C10H1	Isogua	266.086	266.087			
	3N5O5	nosine	2	6	1.23	POS	5.26
		3-(6-A					
		minopu					
		rin-9-y					
543		l)-5-(hy					
		droxym					
		ethyl)c					
		yclopen					
	C11H1	tane-1,2	266.122	266.123			
	5N5O3	-diol	2	5	1.22	POS	4.88
544	C17H1	Persico	297.075	297.076			
	6O6	genin	9	1	8.97	NEG	0.67
545	C15H1	alpha-S	269.119	269.117			
	8O3	antonin	2	0	7.47	POS	-8.17
		3,4-Dim					
546		ethylbe					
	C9H10	nzoic a	299.134	299.131			
	O2	cid	1	5	7.34	NEG	-8.69
547	C15H1	Geniste	271.060	271.060			
	0O5	in	3	2	6.84	POS	-0.37
		S-4-Hy					
548		droxym					
	C12H1	epheny	273.059	273.061			
	4N2O3	toin	4	5	5.07	POS	7.69
		Protosa					
549	C15H1	ppanin	273.074	273.075			
	2O5	A	9	3	5.07	POS	1.46
550	C14H2	N,N,O-	274.116	274.118	4.22	POS	6.57

551	1NO2	Trides methyl venlafa xine 1-Meth yl-6-ox o-1,6-di hydrop yridine -3-carb	8	6			
	C7H7N	oxylic	305.083	305.080			
552	O3	acid	9	9	2.33	NEG	-9.83
	C18H1	Tanshi	277.085	277.085			
553	2O3	none I (1R,4E, 9E,11S) -4,12,12 -trimet hyl-8-o xobicyc lo[9.1.0] dodeca- 4,9-die	5	7	10.98	POS	0.72
	C17H2	n-2-yl	277.179	277.179			
554	4O3	acetate Prohyd rojasmo	0	4	10.47	POS	1.44
	C15H2	n race	277.181	277.179			
555	6O3	mate	8	6	11.22	POS	-7.94
	C12H1		307.061	307.060			
	6O7	Arbutin	8	4	1.33	NEG	-4.56

556		5-Hydr oxymet hyldeo xycytid ine mo					
	C10H1	nophos	280.092	280.091			
557	5N3O5	phate	8	6	0.78	POS	-4.28
	C10H1	Kinsen	282.117	282.118			
558	6O8	oside	9	1	0.91	POS	0.71
	C15H1	Batatasi	283.077	283.075			
559	6O3	n IV	3	2	8.33	POS	-7.42
	C14H1	Maculo	283.109	283.107			
560	6N2O3	sin	9	6	4.45	POS	-8.12
	C17H1	Pendul	315.086	315.086			
561	6O6	one	2	8	7.74	NEG	1.90
	C14H1	Lentici	285.095	285.097			
562	8N2O2	n	8	9	4.12	POS	7.37
	C10H2	Voglibo	285.167	285.166			
563	1NO7	se	0	3	0.84	POS	-2.45
		Dihydr					
564	C16H1	otamari	317.065	317.066			
	4O7	xetin	3	0	5.69	NEG	2.21
565		4-(5-iso propox y-2-Met hyl-4-ni trophen					
	C15H1	yl)pyri	317.112	317.113			
565	6N2O3	dine	5	4	7.89	NEG	2.84
	C20H3	Isostevi	317.210	317.211			
	0O3	ol	6	4	11.23	NEG	2.52

566	C16H1	Licocha	287.090	287.091			
	4O5	lcone B Epoxy	8	1	6.02	POS	1.04
567	C15H2	micheli	287.124	287.124			
	0O4	olide 3 Hydr	2	8	6.12	POS	2.09
568	C9H6O	oxycou	323.057	323.056			
	3	marin 3'-Hydr oxypter	7	9	5.92	NEG	-2.48
569	C16H1	ostilben	295.093	295.093			
	6O4	e	3	7	8.51	POS	1.36
570	C17H1		329.065	329.065			
	4O7	Tricin	2	9	5.88	NEG	2.43
571	C17H1		329.065	329.066			
	4O7	Cirsiliol	3	0	7.09	NEG	2.13
572	C18H1	(±)-Aeg	298.142	298.143			
	9NO3	eline N-cis-C affeoylt	6	2	7.62	POS	2.01
573	C17H1	yramin	300.122	300.122			
	7NO4	e	4	7	5.28	POS	1.00
574	C17H1	Flavoka	301.106	301.106			
	6O5	win C	3	7	9.47	POS	1.33
575	C15H1		303.049	303.049			
	0O7	Morin	1	5	6.16	POS	1.32
576	C21H2	Bavach	337.143	337.143			
	2O4	alcone	1	8	10.97	NEG	2.08
577	C20H3	Pimaric	303.231	303.231			
	0O2	acid	0	4	12.83	POS	1.32
578	C13H1	Orcinol	304.135	304.137	4.13	POS	5.92

	8O7	glucos	5	3			
		ide					
579	C16H1	Tectoch	307.036	307.036			
	2O4	rysin	3	5	10.49	POS	0.65
580	C16H1	Calycos	307.057	307.057			
	2O5	in	1	4	6.22	POS	0.98
581	C20H1	Paulow	351.086	351.086			
	8O7	nin	3	6	10.33	NEG	0.85
		Tanshi					
582	C19H1	none II	317.114	317.114			
	8O3	A	0	4	11.73	POS	1.26
583	C20H3	Lathyro	317.209	317.210			
	0O4	l	1	4	9.19	POS	4.10
		Licocha					
584	C21H2	lcone	353.137	353.138			
	2O5	D	8	6	8.94	NEG	2.27
585	C20H3	Paullini	355.283	355.284			
	8O2	c acid	4	4	14.86	NEG	2.81
		Dihydr					
586	C15H1	omyric	321.060	321.060			
	2O8	etin	9	7	4.87	POS	-0.62
		Lactobi					
587	C12H2	onic ac	357.101	357.102			
	2O12	id	7	8	0.86	NEG	3.08
588	C20H2	Sinacti	322.141	322.143			
	1NO4	ne	9	1	5.05	POS	3.73
		Dibutyl					
589	C18H3	decan	359.245	359.244			
	4O4	edioate	4	6	12.95	NEG	-1.95
590	C18H1	TRIPH	327.076	327.077			
	5O4P	ENYL	8	4	10.84	POS	2.14

		PHOSP					
		HATE					
591	C19H1	Deslora	328.158	328.157			
	9ClN2	tadine	1	8	4.88	POS	-0.91
		Luteoli					
		n 7,3',4'					
592		-trimet					
	C18H1	hyl eth	329.101	329.101			
	6O6	er	6	8	10.11	POS	0.61
593	C20H1	Irisflore	367.075	367.078			
	8O8	ntin	8	8	8.51	NEG	8.17
		5-Ferul					
594	C17H2	oylquin	367.101	367.102			
	0O9	ic acid	1	3	4.28	NEG	3.27
595	C22H2	Gomisi	367.153	367.154			
	6O6	n M2	7	1	10.72	NEG	1.09
		Paeonif					
596	C17H1	lorigen	336.145	336.144			
	8O6	one	4	8	7.23	POS	-1.78
597	C20H1	Glabro	337.100	337.103			
	6O5	ne	8	9	10.33	POS	9.49
		CEPHA					
598	C18H2	LOTAX	338.131	338.134			
	1NO4	INE	7	0	4.00	POS	6.80
		4'-O-bet					
		a-D-Gl					
599		ucosyl-					
		cis-p-co					
	C15H1	umarat	371.096	371.097			
	8O8	e	4	4	3.85	NEG	2.69
600	C16H2	Swerosi	341.121	341.122	4.69	POS	2.64

601	2O9	de	9	8			
		Nepsilo					
		n-Acety					
	C8H16	l-L-lysi	375.231	375.228			
602	N2O3	ne	9	4	0.84	NEG	-9.33
	C20H2	Isocory	376.131	376.132			
	3NO4	dine	9	0	4.58	NEG	0.27
603		Dihydr					
	C21H3	ocortiso	347.218	347.220			
	2O5	l	9	6	7.43	POS	4.90
604		Cheilan					
	C19H1	thifolin	348.115	348.118			
	9NO4	e	6	1	4.51	POS	7.18
605		Shanzh					
		iside m					
	C17H2	ethyl e	387.128	387.128			
606	6O11	ster	3	7	4.03	NEG	1.03
	C22H2	Quassi	387.180	387.180			
	8O6	n	5	9	6.95	NEG	1.03
607		Isoxant					
		hohum					
	C21H2	ol(Soph	355.148	355.151			
608	2O5	ora)	2	1	8.06	POS	8.17
	C18H2	Senecip	356.150	356.148			
	3NO5	hylline	9	9	4.65	POS	-5.62
609	C20H3	KIREN	356.277	356.278			
	4O4	OL	5	5	6.14	POS	2.81
		1-O-alp					
610		ha-D-G					
	C12H2	lucopyr	362.166	362.166			
	4O11	anosyl-	9	3	0.91	POS	-1.66

		D-man					
		nitol					
611	C15H2	Danmel	363.123	363.125			
	2O10	ittoside	0	8	1.62	POS	7.71
		Dimeth					
612	C23H2	ylcurcu	395.154	395.152			
	4O6	min	0	0	10.88	NEG	-5.06
613	C19H1	Daphn	397.049	397.053			
	2O7	oretin	7	1	7.21	NEG	8.56
614	C18H2	Regalos	399.127	399.128			
	4O10	ide A	4	6	4.68	NEG	2.76
		(+)-De					
		methox					
615	C21H2	yascha	371.148	371.148			
	2O6	ntin	7	8	9.55	POS	0.27
616	C17H2	Morron	405.139	405.139			
	6O11	iside	2	7	3.89	NEG	1.23
		Vallesia					
617	C21H2	chotam	373.148	373.150			
	2N2O3	ine	1	2	9.62	POS	5.63
		(19R)-1					
		3-Deox					
618		y-19-hy					
	C20H2	droxye	407.169	407.170			
	6O6	nmein	5	3	5.53	NEG	1.96
		Rhodoj					
619	C22H3	aponin	409.221	409.222			
	4O7	II	3	2	5.90	NEG	2.44
		Glauco					
620	C22H3	calyxin	419.200	419.204			
	0O5	B	7	1	7.89	NEG	8.11

621	C24H3	Resibuf	385.236	385.236	9.57	POS	1.56
	2O4	ogenin Methyl	1	7			
622	C17H2	chloro	386.145	386.145	5.01	POS	-1.55
	0O9	genate	8	2			
623	C22H2	Tetracy	425.140	425.137	4.92	NEG	-6.35
	4N2O8	cline	3	6			
624	C20H2		387.173	387.175	3.97	POS	5.17
	8O6	Phorbol	8	8			
625		2-(10-H eptadec enyl)-6- hydrox			14.74	POS	7.65
	C24H3	ybenzoi	392.309	392.312			
626	8O3	c acid	9	9	4.17	POS	0.76
	C16H1	Magnol	393.057	393.057			
627	8O9	ioside	6	9	8.00	NEG	6.43
	C26H3	Desoxy	435.175	435.178			
628	0O7	limonin Peuced	2	0	4.60	NEG	2.29
	C20H2	anoside	437.106	437.107			
629	2O11	A Mulber	9	9	6.19	NEG	1.59
	C24H2	roside	439.137	439.138			
630	6O9	C	9	6	6.81	NEG	5.92
	C27H3	Ganola	439.243	439.245			
631	8O6	ctone B (-)-Epic atechin	2	8	4.86	NEG	2.72
	C22H1	3-O-ga	441.080	441.081			
	8O10	llate	3	5			

632	C22H2	Liriores	401.157	401.159			
	6O8	inol A	9	0	6.29	POS	2.74
		Deoxyg					
633	C23H2	omisin	401.194	401.195			
	8O6	A	7	3	11.89	POS	1.50
634	C24H3	Phyllan	401.231	401.232			
	4O6	thin	4	1	10.58	POS	1.74
		5-Ethox					
635	C23H3	y-10-Gi	401.265	401.265			
	8O4	ngerol	2	7	12.28	POS	1.25
		3,5,6,7,					
		8,4'-He					
636		xameth					
	C21H2	oxyflav	403.140	403.139			
	2O8	one	3	5	10.02	POS	-1.98
637	C22H2	(+)-Eud	404.202	404.204			
	6O6	esmin	4	6	8.61	POS	5.44
638	C20H1	Molucc	409.088	409.088			
	8O8	anin	0	7	6.14	POS	1.71
639	C23H2	Isolindl	459.128	459.128			
	6O11	eyin	7	9	5.26	NEG	0.44
		6-Hydr					
		oxylute					
640		olin 7-					
	C21H2	glucosi	463.086	463.087			
	0O12	de	6	4	4.67	NEG	1.73
641	C12H1	Armilla	467.105	467.101			
	0O5	risin A	0	7	5.26	NEG	-7.06
		Soyasa					
642	C30H5	pogeno	473.362	473.362			
	0O4	l A	2	9	10.72	NEG	1.48

643	C25H3	Diverso	475.196	475.196			
	4O10	side	2	5	6.39	NEG	0.63
644	C25H2	Mulber	423.174	423.177			
	6O6	rin	4	3	10.33	POS	6.85
645		Geniste					
		in 7-O-					
	C21H2	glucosi	477.102	477.103			
	0O10	de	9	4	5.10	NEG	1.05
646		Oleanol					
	C30H4	ic alde	423.360	423.361			
	8O2	hyde	3	5	14.73	POS	2.83
		Quercet					
647		agetin					
	C21H2	7-glucoside	479.081	479.082			
	0O13	side	1	1	4.56	NEG	2.09
		Laricitr					
648	C22H2	in 3-gl	493.097	493.098			
	2O13	ucoside	4	1	4.66	NEG	1.42
649		Atracty					
	C21H3	loside	493.227	493.228			
650	6O10	A	0	0	3.92	NEG	2.03
	C23H2	Schisan	434.214	434.215			
	8O7	drol B	5	9	9.85	POS	3.22
		4,5-Di-					
651		O-caffe					
	C25H2	oylquin	497.114	497.111			
652	4O12	ic acid	0	2	5.18	NEG	-5.63
	C21H2	Neoliq	436.158	436.159			
	2O9	uiritin	4	3	4.88	POS	2.06
653	C31H4	Poricoi	497.325	497.326			
	6O5	c acid	0	1	10.98	NEG	2.21

		A					
		7-O-Me					
654	C20H2	thylma	437.107	437.107			
	0O11	ngiferin	0	4	4.74	POS	0.92
	C28H2	Viniferi	499.134	499.137			
655	2O6	n	8	3	5.34	NEG	5.01
		2(3H)-F					
		uranon					
		e, 3-((4					
		-(b-D-gl					
		ucopyr					
		anosylo					
		xy)-3-m					
		ethoxy					
		phenyl)					
656		methyl)					
		dihydr					
		o-4-((4-					
		hydrox					
		y-3-met					
		hoxyp					
		enyl)m					
		ethyl)-,					
	C26H3	(3R,4	501.175	501.176			
	2O11	R)-	8	0	5.59	NEG	0.20
	C18H2	Regalos	439.120	439.120			
657	4O11	ide C	5	8	4.08	POS	0.68
	C23H2	Gomisi	439.172	439.172			
658	8O7	n O	1	4	10.43	POS	0.68
	C22H1	(-)-Gall	503.076	503.079			
659	8O11	ocatech	1	6	4.45	NEG	6.96

		in galla					
		te					
		7-Meth					
660	C16H1	oxyflav	503.143	503.146			
	2O3	one	0	5	9.14	NEG	6.96
661	C30H4	gypsog	505.315	505.312			
	6O4	enin	2	1	11.14	NEG	-6.13
662	C30H4	Alisol	507.330	507.327			
	8O4	G	3	5	11.71	NEG	-5.52
		(25R)-S					
663		pirost-4					
	C27H3	-en-3,12	444.307	444.309			
	8O4	-dion	8	3	11.78	POS	3.38
		Alpha-					
664		Tocoph					
	C29H5	erolqui	447.382	447.382			
	0O3	none	5	9	14.53	POS	0.89
		steviol-					
665		19-O-be					
	C26H4	ta-D-gl	515.231	515.236			
	0O8	ucoside	5	6	8.42	NEG	9.90
666	C20H2	Rosavi	451.156	451.157			
	8O10	n	5	0	4.75	POS	1.11
667	C27H4	Pennog	453.288	453.293			
	2O4	enin	9	2	12.32	POS	9.49
		Asperu					
668	C18H2	loside	455.115	455.115			
	4O12	acid	2	6	4.26	POS	0.88
669	C21H2	Isohem	457.111	457.111			
	2O10	iphloin	5	0	4.86	POS	-1.09
670	C21H1	Scutella	463.086	463.087	4.88	POS	0.22

671	8O12	rein 7- glucuro nide Dehydr oandro graphol ide suc	9	0			
	C28H3	cinic ac	531.221	531.222			
	6O10	id 3-O-ace tyl-beta	4	5	8.52	NEG	2.07
672	C32H5	-boswel	533.335	533.337			
	0O4	lic acid	4	9	10.43	NEG	4.50
673	C30H4	Alisol	469.329	469.330			
	6O5	C 7-O-eth	8	8	9.54	POS	2.13
674	C19H3	yl-Morr	473.145	473.143			
	0O11	oniside Cyclog	6	8	5.21	POS	-3.80
675	C30H5	alegeni	473.357	473.360			
	0O5	n	4	3	10.18	POS	5.92
676	C20H2	Folinic	474.172	474.172			
	3N7O7	acid Formon onetin 7-O-xyl	4	8	3.78	POS	0.84
677		osyl-(1					
	C27H3	->6)-gl	543.157	543.153			
	0O13	ucoside	5	9	5.32	NEG	-6.63
678	C23H2	Iristect	475.121	475.123			
	4O12	orin A	9	0	4.95	POS	2.32

679		4'-O-b- D-gluc osyl-5- O-meth					
	C22H2	ylvisam	475.156	475.156			
	8O10	minol	1	8	5.17	POS	1.47
680		Isorha mnetin					
	C22H2	3-gluc	479.117	479.118			
	2O12	oside	6	0	5.10	POS	0.83
681		Myricet in 3-ga					
	C21H2	lactosid	481.102	481.099			
	0O13	e	1	9	4.57	POS	-4.57
682	C22H2	Agnusi	484.174	484.178			
	6O11	de	9	1	4.59	POS	6.61
683		Alisol C 23-ac					
	C32H4	etic aci	563.319	563.317			
	8O6	d	7	1	10.09	NEG	-4.62
684		Caulop hylloge					
	C30H4		489.357	489.357			
	8O5	nin	5	5	9.84	POS	0.00
685		6-O-Ap iosyl-5- O-Meth					
	C27H3	ylvisam	565.190	565.191			
	6O14	mioside	9	5	4.82	NEG	1.06
686		Pinores inol 4-					
	C26H3		565.192	565.192			
	2O11	O-beta-	5	6	5.06	NEG	0.18

		D-glucopyranoside					
687	C29H44O12	Ouabain	565.2661	565.2655	4.74	NEG	-1.06
688		Iristectorigenin B 7-					
	C23H24O12	O-glucoside	493.1329	493.1335	5.25	POS	1.22
689		Alisol F 24-acetate					
	C32H50O6		565.3365	565.3333	10.52	NEG	-5.66
690	C28H38O6	Withanolide A	493.2636	493.2598	8.97	POS	-7.70
691		11-Deoxyxylisol B					
	C30H48O3		495.3331	495.3283	13.38	POS	-9.69
692	C30H48O4	Momordicine I	495.3443	495.3444	10.92	POS	0.20
693		Alisol A 24-acetic acid					
	C32H52O6		567.3514	567.3486	11.06	NEG	-4.94
694	C17H19NO3	Piperine	569.2751	569.2704	9.31	NEG	-8.26
695	C25H41NO9	Aconine	500.2774	500.2814	3.85	POS	8.00
696	C27H34O11	Phillyrin	579.2049	579.2066	5.84	NEG	2.94
697	C29H38	Homoh	580.224	580.228	5.05	NEG	6.55

698	9NO9	arringt online 8-Epi-L oganic acid-6'- O-beta-	3	1			
	C22H3	D-gluc	583.181	583.184			
	4O15	oside 3-O-Ac	0	5	3.95	NEG	6.00
699	C28H3	etylbuf	504.300	504.298			
700	8O7	otalin	6	1	10.48	POS	-4.96
	C30H4	bayoge	511.340	511.339			
	8O5	nin Genipi n 1-bet	0	7	10.14	POS	-0.59
701		a-genti					
702	C23H3	obiosid	595.187	595.187			
	4O15	e Quercet in 3-(2'' -galloyl	8	9	4.15	NEG	0.17
	C28H2	galacto	597.093	597.090			
703	4O16	side)	3	7	4.95	NEG	-4.35
	C28H3	Kakkali	607.166	607.166			
	2O15	de	5	7	5.67	NEG	0.33
704	C29H2	Neothe	609.121	609.123			
705	4O12	aflavin	6	3	5.22	NEG	2.79
	C27H3		609.143	609.144			
	0O16	Rutin	3	7	4.74	NEG	2.30
706	C27H2	Doxoru	526.181	526.176			
	9NO11	bicin	8	6	5.58	POS	-9.88

		Termin					
707	C30H4	olic aci	527.333	527.334			
	8O6	d	8	1	8.60	POS	0.38
		Gymne					
708	C30H5	mageni	529.356	529.353			
	0O6	n	0	0	6.75	POS	-5.67
709	C30H3	Toosen	619.238	619.238			
	8O11	danin	2	9	7.59	NEG	1.13
		Angelo					
710	C28H3	ylgomi	539.204	539.204			
	6O8	sin H	2	2	10.37	POS	0.00
		Secoiso					
		laricires					
711		inol m					
	C26H3	onoglu	547.214	547.214			
	6O11	coside	8	9	4.68	POS	0.18
712	C28H3	Gomisi	548.249	548.249			
	4O10	n D	0	0	9.64	POS	0.00
		Chrysi					
		n 6-C-a					
		lpha-L-					
713		arabino					
		pyrano					
		side-8-					
	C26H2	C-gluco	549.160	549.160			
	8O13	side	5	4	4.80	POS	-0.18
		Pseudo					
		laric A					
714		cid A-					
	C28H3	O-beta-	551.242	551.245			
	8O11	D-gluc	9	8	7.87	POS	5.26

		opyran					
		oside					
715	C30H2	Tilirosi	639.123	639.129			
	6O13	de	6	6	6.02	NEG	9.39
716	C33H5		559.361	559.362			
	2O8	Trillin	7	6	11.10	POS	1.61
717	C30H3	Tenuifo	649.177	649.177			
	6O17	lisode B	3	1	4.86	NEG	-0.31
		Euphor					
718	C30H3	bia fact	562.225	562.222			
	7NO7	or L8	2	7	11.07	POS	-4.45
719	C28H3	Hesperi	655.186	655.187			
	4O15	din	5	2	5.20	NEG	1.22
720	C26H3	Cassias	567.171	567.170			
	0O14	ide B	0	9	5.94	POS	-0.18
		Pachy					
721	C33H5	mic aci	567.354	567.349			
	2O5	d	2	4	12.43	POS	-8.46
		Ligustr					
722	C25H3	osidic	572.208	572.203			
	0O14	acid	6	0	5.00	POS	-9.79
		Arenob					
723		ufagin					
	C32H4	3-hemis	573.301	573.303			
	4O9	uberate	7	8	9.49	POS	3.49
724	C27H3	Isorhoif	579.171	579.170			
	0O14	olin	0	9	5.03	POS	-0.17
725	C32H4	Clemas	683.251	683.253			
	4O16	taninB	5	6	4.53	NEG	3.07
726	C27H3	Kaempf	595.166	595.166			
	0O15	erol 3-	2	0	4.79	POS	-0.34

		neohes					
		peridos					
		ide					
		6'-Ferul					
727	C30H3	oylnod	602.223	602.223			
	2O12	akenin	8	5	6.32	POS	-0.50
		Episyri					
		ngaresi					
		nol 4'-					
728		O-beta-					
		D-glnco					
	C28H3	pyrano	603.203	603.203			
	6O13	side	1	9	5.09	POS	1.49
		3-Ferul					
		oyl-1-Si					
729		napoyl					
	C33H4	sucros	723.209	723.211			
	0O18	e	6	9	5.28	NEG	3.18
		Luteoli					
		n 4'-me					
		thyl et					
730		her 7-r					
	C28H3	utinosi	609.181	609.181			
	2O15	de	0	2	5.13	POS	0.33
		methyl					
		(4S,5Z,					
		6S)-5-et					
731		hyliden					
		e-4-[2-o					
	C31H4	xo-2-	731.236	731.238			
	2O17	[[(2R,3	4	4	4.88	NEG	2.74

		S,4S,5R, 6R)-3,4, 5-trihy droxy-6 -[2-(4-h ydroxy phenyl) ethoxy] oxan-2- yl]meth oxy]eth yl]-6-[(2 S,3R,4S, 5S,6R)- 3,4,5-tri hydrox y-6-(hy droxym ethyl)o xan-2-y l]oxy-4 H-pyra n-3-car boxylat e 4''-O-Gl					
732	C27H3	ucosylv	612.186	612.189			
	0O15	itexin	7	5	4.71	POS	4.57
		3-Deox					
733	C34H4	yaconiti	612.320	612.318			
	7NO10	ne	3	8	7.41	POS	-2.45

734		9-Dihydro-13-acetyl					
	C33H4	accatin	613.258	613.261			
	2O12	III	2	6	8.14	POS	5.54
735		Kouitch					
	C27H3	enside	614.201	614.204			
	2O15	G	5	7	5.21	POS	5.21
736	C34H4	Forsyth	755.238	755.239			
	4O19	oside B	8	6	4.96	NEG	1.06
737		Tarasap					
	C41H6	onin V	763.427	763.427			
	4O13	I	2	3	9.67	NEG	0.13
738		Gentiiri					
	C36H4	dosides	777.224	777.224			
	2O19	A	1	4	5.20	NEG	0.39
739	C41H6	Cogoxi	779.422	779.422			
	4O14	n	7	5	7.02	NEG	-0.26
740	C36H4	Angoro	783.271	783.271			
	8O19	side C	7	7	4.96	NEG	0.00
741		3,4',6'-Trihydroxy-4,2'-dimethoxychalcone 4'					
	C29H3	-O-ruti	647.193	647.194			
	6O15	noside	6	1	5.60	POS	0.77
742		Kaempferol 3-s					
	0O21	ophoro	0	7	4.07	NEG	2.08

		side-7-g lucosid e					
743	C19H2		819.230	819.232			
	2O10	aloenin	1	7	5.05	NEG	3.17
		Epicate chin-(2 beta-> 7,4beta ->8)-epi catechi n-(4bet a->8)-e					
744							
	C45H3	picatec	845.163	845.167			
	6O18	hin	8	8	4.33	NEG	4.73
745	C42H6	Lucyosi	857.454	857.454			
	8O15	de B	0	0	6.43	NEG	0.00
746	C32H3	Camelli	727.206	727.207			
	8O19	aside B	8	4	4.64	POS	0.83
747	C33H4	Troxe	743.239	743.239			
	2O19	utin	1	2	4.65	POS	0.13
	C45H5	Pristina					
748	4N8O1	mycin	911.400	911.397			
	0	IA	7	6	9.36	NEG	-3.40
749	C20H2	Regalos	915.275	915.276			
	6O12	ide E	4	5	4.81	NEG	1.20
		10-Deac etyl-7-x ylosyl					
750							
	C50H5	paclitax	924.327	924.335			
	7NO17	el	6	9	8.58	NEG	8.98

751		Pennog enin 3- O-beta-					
	C45H7	chacotri	929.474	929.475			
	2O17	oside	8	0	9.21	NEG	0.22
752	C47H7	Celosin	939.455	939.457			
	4O20	L	4	2	6.60	NEG	1.92
753	C46H7		950.498	950.493			
	7NO17	Tylosin	9	7	6.60	NEG	-5.47
754		20(R)-G insenos					
	C42H7	ide Rg	767.487	767.490			
	2O13	2	0	8	7.37	POS	4.95
755		Carbox					
	C31H4	yatract	771.205	771.212			
	6O18S2	yloside	0	4	4.94	POS	9.60
756		Notogi					
	C47H8	nsenosi	967.499	967.501			
	0O18	de R1	2	5	5.41	NEG	2.38
757	C47H8	Hosenk	983.494	983.496			
	0O19	oside F	6	7	4.94	NEG	2.14
758	C41H6	Bacopa	784.480	784.482			
	6O13	side V	8	5	8.49	POS	2.17
759	C48H7	Asiatic	1009.47	1009.47			
	8O20	oside B	86	83	5.37	NEG	-0.30
760	C25H3	Picrosi	1075.32	1075.32			
	0O13	de III	86	93	4.74	NEG	0.65
761		Deapio					
	C52H8	platyco	1091.52	1091.52			
	4O24	din D	62	71	6.04	NEG	0.82
762	C42H6	Eclalba	819.450	819.450	7.04	POS	0.00

	8O14	saponin I 11-Oxo	1	1			
763	C42H7 0O14	mogros ide IIe 4-O-gal	821.466 4	821.466 1		6.22 POS	-0.37
764	C30H3 2O15	loylalbi florin Fructo- oligosa ccharid	1263.36 33	1263.35 21		5.19 NEG	-8.87
765	C48H8 2O41	e DP8/ GF7 Liriope Musca ri baily	1349.39 29	1349.39 78		0.96 NEG	3.56
766	C44H7 0O17	Sapon ins C ilexsap	888.510 7	888.502 9		9.55 POS	-8.78
767	C47H7 6O17	onin B 2	895.507 8	895.506 7		7.77 POS	-1.23
768	C48H7 8O19	Isoasiat icoside Alpha-c	941.515 6	941.513 3		5.45 POS	-2.44
769	C36H6 0O30	yclodex trin	995.305 2	995.305 7		1.05 POS	0.50
770	C53H8 4O23	Aralosi de C	1071.54 30	1071.54 03		6.90 POS	-2.52
771	C51H8 2O24	Terrestr osin K	1101.50 32	1101.50 60		5.96 POS	2.54
772	C58H9	Celosin	1217.55	1217.55		6.74 POS	2.63

	0028	J	28	60			
		3-Hydr					
		oxybut					
773	C4H8O	3-Butyric acid	103.039	103.039			
	3		5	8	1.50	NEG	2.91
		METH					
		ACRYL					
774	C4H6O	2-Butyric acid	104.071	104.071			
	2		4	0	0.84	POS	-3.84
		alpha-					
		Amino					
775	C4H9N	2-Butyric acid	104.071	104.070			
	O2		2	9	1.05	POS	-2.88
		2-hydro					
		xyethyl					
776		(propa					
	C5H14	n-2-yl)an	104.107	104.107			
	NO+	zanium	8	4	0.83	POS	-3.84
		2-(Isopr					
		opylam					
777	C5H13	ino)eth	104.107	104.107			
	NO	anol	6	3	1.20	POS	-2.88
		Hexa-2,					
778	C6H6O	4-diene	109.029	109.029			
	2	dial	1	3	3.40	NEG	1.83
		5-meth					
		ylol-3H					
779	C5H6O	-furan-	113.024	113.024			
	3	2-one	0	2	0.79	NEG	1.77
780	C8H12	cyclope	121.066	121.065			
	O2	ntanon	1	7	5.53	NEG	-3.30

781		e, 3-(2-oxopro pyl)- 3-Meth yl-2-cyc lopente	114.092	114.091			
	C6H8O	n-1-one	1	7	4.04	POS	-3.51
782	C6H6O	Pyrogal	125.024	125.024			
	3	lol	0	2	2.12	NEG	1.60
783		DL-Ho moseri	120.065	120.065			
	O3	ne	9	7	0.88	POS	-1.67
784		cis-4-H ydroxy	130.050	130.050			
	O3	proline	1	5	1.18	NEG	3.84
785		4-Hydr oxy-2-p yrrolidi necarbo					
	C5H9N	xylic a	130.050	130.050			
786	O3	cid	2	6	0.90	NEG	3.08
		(±)-eryt hro-Isol	130.086	130.087			
787	NO2	eucine	6	0	1.48	NEG	3.07
	C5H10	DL-Glu	129.065	129.066			
788	N2O3	tamine	8	1	0.86	POS	2.32
	C5H9N	DL-Glu	130.049	130.049			
789	O4	tamate	3	9	0.90	POS	4.61
		methyl pyrogl	142.050	142.050			
	O3	utamat	2	6	1.43	NEG	2.82

		e					
790	C5H7N	jatroph	131.082	131.082			
	O2	am	5	0	1.41	POS	-3.81
791	C5H14	Agmati	131.129	131.129			
	N4	ne	5	3	0.73	POS	-1.53
792	C6H14		145.097	145.098			
	N2O2	Lysine	7	0	0.76	NEG	2.07
		5-Hydr					
793	C8H7N	oxyoxi	132.044	132.044			
	O2	ndole	2	6	4.07	POS	3.03
		3-Hydr					
794	C5H9N	oxyprol	132.067	132.066			
	O3	ine	9	7	0.85	POS	-9.09
		p-Hydr					
795		oxypro					
	C9H10	piophe	133.064	133.064			
	O2	none	0	7	5.26	POS	5.26
		1-Deox					
796	C6H14	y-D-glu	147.066	147.066			
	O5	citol	3	0	1.53	NEG	-2.04
797	C4H7N	Asparti	134.045	134.044			
	O4	c acid	0	9	0.67	POS	-0.75
798	C5H10	D-Apio	149.044	149.045			
	O5	se	5	0	0.89	NEG	3.35
799	C10H1	Sobrepi	151.112	151.112			
	8O2	n	7	5	7.11	NEG	-1.32
		2,5-dim					
800		ethylbe					
	C9H10	nzalde	135.080	135.080			
	O	hyde	6	5	4.69	POS	-0.74
801	C10H1	p-Cym	135.116	135.116	7.57	POS	0.00

	4	ene	8	8			
		Tert-bu					
802	C10H1	tylbenz	135.117	135.117			
	4	ene	2	0	4.49	POS	-1.48
803	C8H11	Octopa	136.075	136.075			
	NO2	mine	1	7	1.25	POS	4.41
		dehydr					
804	C6H6O	oascorb	154.998	154.998			
	6	icacid	4	2	1.00	NEG	-1.29
		5-(meth					
		oxymet					
805		hyl)fur					
		an-2-ca					
	C7H8O	rboxyli	155.034	155.034			
	4	c acid	2	6	5.08	NEG	2.58
		Parasor					
806	C6H8O	bic aci	157.049	157.050			
	2	d	8	2	4.60	NEG	2.55
		3-MET					
		HYL-1,					
807		2-CYCL					
		OPENT					
	C6H12	ANEDI	161.081	161.081			
	O2	OL	3	6	4.82	NEG	1.86
		(1R,2R,					
		3S)-3-m					
808		ethylcy					
		clopent					
	C6H12	ane-1,2-	161.081	161.081			
	O2	diol	1	5	4.26	NEG	2.48
809	C6H6O	epimed	143.034	143.034	3.70	POS	-1.40

	4	okorea	3	1			
		none A					
		1,2,4-Tr					
810		ihydrox					
	C6H6O	ybenze	144.065	144.065			
	3	ne	7	6	1.75	POS	-0.69
		threono					
811	C4H6O	-1,4-lact	163.024	163.024			
	4	one	2	5	0.90	NEG	1.84
		2-(2,3,4-					
		trihydr					
812		oxyphe					
	C8H7N	nyl)acet	164.034	164.035			
	O3	onitrile	7	0	3.46	NEG	1.83
		2,3,4,5-t					
		etrahyd					
813		roxype					
	C5H10	ntanoic	165.039	165.040			
	O6	acid	5	0	0.84	NEG	3.03
814	C9H6O	Chrom	147.043	147.043			
	2	one	7	9	1.25	POS	1.36
		4-hydro					
		xy-2-m					
815		ethoxy					
	C8H8O	benzoic	167.034	167.034			
	4	acid	0	5	4.48	NEG	2.99
		3-hydro					
		xy-vani					
816	C8H10	llic aci	167.034	167.034			
	O5	d	8	6	2.86	NEG	-1.20
817	C11H9	2-Meth	168.045	168.045	5.21	NEG	-0.60

	NO2	yl-N-ph	1	0			
		enylma					
		leimide					
		2-Cyclo					
818	C8H12	octenon	169.086	169.086			
	O	e	4	7	7.59	NEG	1.77
		Di-2-fu					
819	C9H8O	ranylm	149.059	149.059			
	2	ethane	7	7	2.25	POS	0.00
		BIHEP					
		TADIE					
820		NECA					
		RBOXY					
	C7H10	LIC A	171.065	171.065			
	O2	CID	3	8	5.33	NEG	2.92
		7-Meth					
821	C6H7N	yladeni	150.078	150.078			
	5	ne	6	0	1.17	POS	-4.00
822	C7H13	Norhyg	172.097	172.097			
	NO	rine	1	5	4.64	NEG	2.32
		(-)-Nor					
823	C9H13	ephedri	152.106	152.106			
	NO	ne	8	9	1.51	POS	0.66
		1, 7, 7-					
		Trimet					
824		hylbicy					
		clo[2.2.					
		1]hept-					
	C10H1	5-en-2-	153.127	153.127			
	6O	ol	2	3	7.57	POS	0.65
825	C5H9N	4-Amin	154.026	154.026	0.83	POS	0.00

826	O2	o-2-met hyleneb utanoic acid (E)-4-h ydroxy hex-2-e	5	5			
	C6H10	noic ac	175.060	175.060			
827	O3	id	4	8	4.17	NEG	2.28
	C12H2	Alepryl	177.128	177.128			
828	0O2	ic acid	3	1	8.97	NEG	-1.13
	C4H6O	Malic a	179.018	179.019			
829	5	cid suspen	9	3	0.89	NEG	2.23
	C10H1	olic aci	179.071	179.070			
830	4O4	d Noreca	0	9	6.04	NEG	-0.56
	C11H1	santalic	179.106	179.107			
831	6O2	acid N-amid	8	3	8.60	NEG	2.79
	C6H11	ino-L-p	158.092	158.092			
832	N3O2	roline 2-Hydr oxytere	5	5	0.73	POS	-0.63
	C8H6O	phthali	181.013	181.013			
833	5	c acid 2-Amin	4	8	4.14	NEG	2.76
	C7H7N	obenzoi	182.044	182.045			
834	O2	c acid	9	4	4.27	NEG	2.75
	C7H7N	2-Hydr	182.044	182.045			
	O2	oxyben	9	4	3.40	NEG	2.75

		zaldehy					
		de oxi					
		me					
		Amino					
835	C6H11	adipic	162.075	162.075			
	NO4	acid	3	7	1.17	POS	2.47
836	C6H4O	Cumali	185.008	185.008			
	4	c acid	6	9	1.45	NEG	1.62
		3,7-dih					
837		ydroxy					
	C9H8O	chroma	163.038	163.038			
	4	n-4-one	2	9	3.79	POS	4.29
838	C6H11	pegalin	163.107	163.107			
	NO3	e	3	5	0.67	POS	1.23
839	C11H1	Jasmolo	163.111	163.111			
	6O2	ne	3	8	7.43	POS	3.07
		Couma					
840	C9H8O	rinic ac	165.054	165.054			
	3	id	2	4	1.25	POS	1.21
		trihydr					
841	C10H2	oxyMe	187.133	187.133			
	0O3	nthane	2	6	8.17	NEG	2.14
		Acetop					
842		henone,					
	C10H1	3-ethy	166.122	166.122			
	2O	l-	6	6	1.62	POS	0.00
		Butoxy					
843	C8H14	succinic	189.076	189.076			
	O5	Acid	2	5	4.84	NEG	1.59
844	C8H12	L,L-Cyc	169.096	169.096			
	N2O2	lo(prol	4	8	2.40	POS	2.37

		ylalany					
		l)					
		Methox					
845	C11H1	yeugen	193.086	193.086			
	4O3	ol	0	5	8.34	NEG	2.59
846	C10H1	Damasc	194.081	194.081			
	3NO3	enine	3	8	6.58	NEG	2.58
		N-Acet					
847		yl-DL-g					
	C7H11	lutamic	172.059	172.060			
	NO5	acid	2	1	1.28	POS	5.23
		delta2,4					
		-dihydr					
848		ophthal					
	C8H6O	ic anhy	195.028	195.029			
	3	dride	9	4	4.72	NEG	2.56
		Boschni					
849	C9H14	alacton	172.133	172.133			
	O2	e	0	1	4.99	POS	0.58
		1-Propa					
		none, 3					
		-hydro					
850		xy-1-(4-					
		hydrox					
		y-3-met					
	C10H1	hoxyp	195.065	195.065			
	2O4	enyl)-	5	9	4.02	NEG	2.05
851	C10H1	Piperito	172.169	172.169			
	8O	l	2	4	9.20	POS	1.16
852	C8H13	SCOPO	173.128	173.128			
	NO2	LINE	8	6	2.13	POS	-1.16

853	C6H11	2-Oxo	174.087	174.087			
	N3O3	arginine	1	2	0.95	POS	0.57
854		5,6-dio					
		xocyclo					
855		hexa-1,					
		3-diene					
856		-1-carb					
	C7H4O	oxylic	197.008	197.008			
857	4	acid	4	8	2.80	NEG	2.03
		2-none					
858	C9H16	nic aci	174.149	174.149			
	O2	d	4	1	4.09	POS	-1.72
859	C7H14	theanin	175.107	175.107			
	N2O3	e	7	7	4.43	POS	0.00
860		N-gam					
		ma-L-G					
861		lutamyl					
	C8H14	-D-alan	199.072	199.072			
862	N2O5	ine	1	0	1.47	NEG	-0.50
	C7H13	Calyste	176.091	176.091			
863	NO4	gine B2	5	6	0.91	POS	0.57
		megasti					
864		gma-3,7					
	C13H2	(E),9-tri	177.163	177.163			
865	0	ene	6	7	11.33	POS	0.56
	C7H8O	Daucic	203.018	203.019			
866	7	acid	7	2	0.94	NEG	2.46
		(2-Nap					
867		hthyl)					
	C11H1	methan	203.070	203.071			
	OO	ol	6	0	6.81	NEG	1.97

		Diethyl					
862	C12H1	phthal	203.071	203.071			
	4O4	ic acid	4	1	9.14	NEG	-1.48
		(e)-4-(3,					
		4-dihyd					
863		roxyph					
		enyl)bu					
	C10H1	t-3-en-2	179.070	179.070			
	0O3	-one	1	2	4.69	POS	0.56
		alpha,al					
		pha-Di					
864		methyl					
		phenet					
	C11H1	hyl for	179.106	179.106			
	4O2	mate	7	7	6.02	POS	0.00
	C10H1	(R)-Sals	180.101	180.101			
865	3NO2	olinol	7	8	1.20	POS	0.56
	C10H1		180.102	180.102			
866	0O2	Safrole	7	3	4.04	POS	-2.22
	C11H1	Cantley	206.081	206.081			
867	3NO3	ine	5	9	4.86	NEG	1.94
		6-Meth					
868	C11H1	oxymel	207.065	207.065			
	2O4	lein	5	9	6.85	NEG	1.93
	C9H16	Cyclo(Il	185.128	185.128			
869	N2O2	e-Ala)	6	5	4.45	POS	-0.54
		Ethyl 3					
		-cycloh					
870	C11H2	exylpro	185.153	185.153			
	0O2	pionate	4	5	11.73	POS	0.54
871	C10H9	5-Hydr	209.044	209.045	4.11	NEG	1.91

872	O5-	oxyferu late methyl (1R,4a S,6S,7R, 7aS)-1,6 -dihydr oxy-7- methyl- 1,4a,5,6, 7,7a-he xahydr ocyclop enta[d] pyran-4	7	1				
	C11H1 6O5	-carbox ylate Phenol, 4-(1,1- dimeth ylethyl)	209.081 4	209.081 4		5.28	NEG	0.00
873	C11H1 6O	-2-meth yl- Sedano	209.117 5	209.117 9		8.46	NEG	1.91
	C12H1 8O3	nic aci d N-(3,4,5 -trimet hoxyp	209.117 5	209.117 9		7.63	NEG	1.91
875	C10H1 3NO4	enyl)for mamid	210.076 2	210.076 7		4.48	NEG	2.38

		e					
		methyl					
		2-hydr					
876		oxy-3,4-					
		dimeth					
	C10H1	oxyben	211.060	211.060			
	2O5	zoate	2	7	3.78	NEG	2.37
877	C9H14	ningpo	188.128	188.128			
	O3	genin	1	1	4.72	POS	0.00
		7-hydro					
		xy-6-(2-					
878		hydrox					
		yethyl)					
	C11H1	coumar	189.053	189.054			
	0O4	in	6	4	5.80	POS	4.23
		Cincho					
879		ninic a					
	C10H7	cid, 2-h	190.050	190.050			
	NO3	ydroxy-	3	1	4.11	POS	-1.05
880	C11H1	(-)-Cyti	191.118	191.118			
	4N2O	sine	0	0	1.96	POS	-0.52
		Deoxye					
881	C9H11	ritadeni	218.064	218.066			
	N5O3	ne	8	3	1.25	NEG	6.88
		3-(4-me					
		thoxyp					
882		henyl)-					
		2-meth					
	C11H1	yl-2-acr	193.086	193.086			
	2O3	ylicacid	5	2	4.91	POS	-1.55
883	C12H1	2-Prope	219.065	219.065	6.60	NEG	0.00

884	4O5	noic ac	7	7			
		id, 3- (3,4,5-tr imetho xyphen yl)- 2-(1-ox openty l)-benz oicacid					
885	C13H1	methy	219.101	219.102			
	6O3	l ester	7	2	8.71	NEG	2.28
886	C6H9N	D-Histi	194.032	194.032			
	3O2	dine	4	5	0.78	POS	0.52
887		1-[2-(fu ran-2-y l)-2-oxo ethyl] pyrroli-					
	C10H1	din-2-o	194.081	194.081			
888	1NO3	ne	4	3	4.49	POS	-0.52
		saikoch romicac					
889	C10H6	id	221.008	221.008			
	O6	id	2	7	4.56	NEG	2.26
890		3,4-Dih ydroxy- 5-[(S)-1, 2-dihyd roxyeth yl]fura					
	C6H8O	n-2(5H)	221.029	221.029			
891	6		1	7	0.92	NEG	2.71

		-one					
889	C9H8N	Pemoli	221.056	221.056			
	2O2	ne	0	4	3.53	NEG	1.81
		4,7-Dih					
		ydroxy-					
890		3-butyl					
	C12H1	phthali	221.081	221.081			
	4O4	de	3	6	6.93	NEG	1.36
	C12H1	Ethyl f	221.081	221.081			
891	4O4	erulate	1	5	5.49	NEG	1.81
	C14H2	Kobuso	221.153	221.154			
892	2O2	ne	5	1	9.29	NEG	2.71
		methyl					
		syram					
893	C11H1	uraldeh	223.060	223.060			
	4O6	ydate	7	7	5.20	NEG	0.00
		(E-p-hy					
		droxy-c					
894	C10H1	innami	196.096	196.096			
	0O3	c acid	8	8	3.77	POS	0.00
		Paeonil					
895	C10H1	actone	197.080	197.080			
	2O4	B	4	6	5.28	POS	1.01
	C11H1	isololiol	197.116	197.117			
896	6O3	ide	8	0	5.24	POS	1.01
	C9H11	DL-Do	198.076	198.076			
897	NO4	pa	3	2	1.14	POS	-0.50
		methyl					
		(2S)-3-					
898	C10H1	hydrox	198.112	198.112			
	2O3	y-2-phe	3	4	1.68	POS	0.50

		nylpro					
		panoate					
899	C12H1	FA 12:	225.112	225.113			
	8O4	3+2O	8	0	5.64	NEG	0.89
		p-hydr					
900		oxy-co					
	C9H10	umaric	227.055	227.055			
	O4	acid	5	8	3.80	NEG	1.32
		Cyclod					
901	C12H2	odecan	200.200	200.200			
	2O	one	5	7	10.55	POS	1.00
		8-Hydr					
		oxy-2-					
		methox					
902		y-6-met					
		hyl-1,4-					
		naphth					
	C12H1	oquino	201.053	201.054			
	0O4	ne	6	4	7.57	POS	3.98
		cis-p-m					
903		enth-2-					
	C10H1	ene-1 α ,	231.122	231.123			
	8O3	7,8-triol	8	3	5.47	NEG	2.16
		5-Hydr					
904		oxy-L-t					
	C11H1	ryptop	203.080	203.081			
	2N2O3	han	9	5	1.64	POS	2.95
		2,5-dim					
905		ethyl-4-					
	C9H18	Methox	204.122	204.122			
	NO4+	yphena	4	7	0.92	POS	1.47

		nthrene					
906	C15H2	madoli	233.153	233.154			
	2O2	n w	8	2	8.80	NEG	2.14
		senkyu					
907	C12H1	nolide	205.085	205.086			
	4O4	D	5	0	6.39	POS	2.44
		Octopi					
908	C8H16	nic aci	205.117	205.118			
	N2O4	d	9	1	0.90	POS	0.98
		cis-1-(2-furyl)-4					
909		-(2-thie					
		nyl)-1-b					
	C12H8	uten-3-	235.001	235.000			
	OS	yne	2	1	5.63	NEG	-4.68
		schinic					
910	C12H1	oumari	235.060	235.060			
	2O5	n	2	7	5.41	NEG	2.13
911	C12H1	neoligu	235.096	235.097			
	4O2	stilide	8	2	8.38	NEG	1.70
		Hyalur					
912	C8H15	onic ac	206.101	206.102			
	NO5	id_qt	7	0	0.85	POS	1.46
		senkyu					
913	C12H1	nolide-	207.101	207.101			
	4O3	F	8	7	8.21	POS	-0.48
		2,3-Dih					
914		ydroxy					
		propyl					
	C12H1	3-(4-hy	237.075	237.076			
	4O5	droxyp	8	3	5.10	NEG	2.11

		henyl)p					
		rop-2-e					
		noate					
915	C11H1	Isoshin	237.076	237.076			
	2O3	anolone	0	4	5.93	NEG	1.69
		2-Amin					
		o-4-hyd					
916		roxy-6-					
		pteridi					
		necarbo					
	C7H5N	xylic a	208.046	208.046			
	5O3	cid	5	5	1.60	POS	0.00
917	C11H1	psilotic	208.096	208.096			
	0O3	acid	6	7	1.18	POS	0.48
		corydal					
		dine(ta					
918		utomeri					
	C11H1	cstruct	208.096	208.096			
	3NO3	ure 1)	8	8	5.03	POS	0.00
		3-Hydr					
		oxy-1-					
		(4-hydr					
919		oxy-3,5-					
		dimeth					
		oxyphe					
		nyl)pro					
	C11H1	pan-1-o	209.080	209.080			
	4O5	ne	4	9	4.40	POS	2.39
		Senkyu					
920	C12H1	nolide-	239.091	239.092			
	6O5	R	9	2	5.71	NEG	1.25

		Senkyu					
921	C12H1	nolide	209.117	209.117			
	6O3	G	0	1	8.02	POS	0.48
		2-[(1R)-					
		4-meth					
		yl-1-cyc					
922		lohex-3					
		-enyl]p					
		rop-2-e					
	C12H1	nyl ace	239.127	239.128			
	8O2	tate	9	4	9.74	NEG	2.09
		4-[(E)-3					
		-ethoxy					
		prop-1-					
923		enyl]-2-					
		methox					
	C12H1	ypheno	209.117	209.117			
	6O3	l	2	2	7.27	POS	0.00
		peristro					
924	C9H9N	phamid	240.050	240.051			
	O4	e i	6	0	3.14	NEG	1.67
925	C11H1	Ganoin	240.123	240.123			
	7NO2	e	1	6	5.88	NEG	2.08
		-ethyl					
		3-(4-hy					
926		droxyp					
	C11H1	henyl)a	210.112	210.112			
	2O3	crylate	3	4	7.49	POS	0.48
		senkyu					
927	C12H1	nolide	241.062	241.063			
	5ClO3	L	9	3	8.21	NEG	1.66

928	C10H1	Tubero	211.107	211.107			
	1NO3	sine B	9	8	3.43	POS	-0.47
		Spiroxa					
929	C11H1	bovolid	241.107	241.107			
	6O3	e	1	6	5.05	NEG	2.07
930	C10H1	Cyclo(P	241.118	241.118			
	6N2O2	ro-Val)	4	9	4.62	NEG	2.07
		cyclo					
931	C11H1	(D)-Pro	211.144	211.144			
	8N2O2	-(D)-Ile	1	1	4.93	POS	0.00
		2-Hydr					
932		oxy-3-					
		methyl-					
	C13H1	9H-car	242.081	242.081			
	1NO	bazole	3	8	7.36	NEG	2.07
933	C12H2	cucurbi	213.148	213.148			
	0O3	c acid	3	4	7.37	POS	0.47
934	C14H1	Eriobof	243.065	243.065			
	2O4	uran	2	8	8.58	NEG	2.06
935	C9H14	pedatis	215.102	215.102			
	N2O4	ectine f	4	5	1.43	POS	0.46
		Furano					
936	C15H2	germen	215.142	215.142			
	0O2	one	2	9	9.64	POS	3.25
937	C10H1	ZINC0	216.123	216.123			
	4O4	0394284	6	3	4.13	POS	-1.39
938	C10H1	linamar	246.096	246.097			
	7NO6	in	9	6	4.30	NEG	2.84
		1,2,3,9-t					
939	C12H1	etrahyd	217.097	217.097			
	2N2O2	ropyrro	6	4	4.24	POS	-0.92

		lo(2,1- b)quina zolin-1- carboxy licacid					
940	C10H1 7NO3	Neotus silagine	217.154 7	217.154 7			
		beta-D-			1.87	POS	0.00
941	C6H13 NO5	Galacto samine	218.042 5	218.042 5			
		2,8-dim ethyl-5- acetyl-b			0.75	POS	0.00
942		icyclo [5,3,0]					
	C14H2 OO	deca-di ene-1,8	249.148 6	249.149 1			
		RJNYN DHYSJ RRDW- BUHF			10.35	NEG	2.01
943	C11H9 N3O2	OSPRS A-N	250.037 9	250.038 4			
					1.24	NEG	2.00
944	C11H1 1NO3	doryph ornine	250.070 9	250.071 5			
		8,9-Dih ydroxy- 1,5,6,10 B-tetra			4.64	NEG	2.40
945	C12H1 3NO3	hydrop yrrolo	220.096 8	220.096 8			
					4.69	POS	0.00

		[2,1-A]i					
		soquin					
		olin-3(2					
		H)-one					
946	C11H1	vinyl c	251.055	251.055			
	0O4	affeate	1	6	6.04	NEG	1.99
		7,3',4'-tr					
		ihydrox					
947		y-3-ben					
		zyl-2H-					
	C16H1	chrome	251.071	251.071			
	4O4	ne	2	0	6.05	NEG	-0.80
		(z)-6,7-					
		epoxy-					
948		6,7-dih					
	C12H1	ydrolig	251.091	251.091			
	4O3	ustilide	3	9	8.24	NEG	2.39
	C10H1	D-Kyn	253.082	253.082			
949	2N2O3	urenine	2	6	2.13	NEG	1.58
	C11H1	terrestri	255.086	255.086			
950	4O4	c acid	4	9	4.78	NEG	1.96
	C16H1	Rutacul	255.102	255.102			
951	8O4	tin	3	2	10.01	NEG	-0.39
		plantag					
		oguani					
952	C11H1	dinic,ac	226.154	226.154			
	9N3O2	id	6	8	1.27	POS	0.88
		(6R, 7					
		E)-9-hy					
953	C13H2	droxy-	226.179	226.179			
	0O2	4, 7-me	4	8	7.15	POS	1.77

		-gastig madien -3- one 9H-xan thene-2 -carbox					
954	C14H1 0O3	ylic aci d	227.069 7	227.070 0			
					7.57	POS	1.32
955	C10H1 4N2O4	Carbid opa	227.102 8	227.102 7			
					2.79	POS	-0.44
956	C12H1 8O4	erigere none b	227.127 0	227.127 4			
					9.74	POS	1.76
		2-(1-eth oxy-2-h ydroxy) propyl- 4-meth					
957	C12H1 8O4	oxyphe nol(i)	227.127 0	227.127 4			
					5.34	POS	1.76
		DL-Pyr ogluta					
958	C5H7N O3	mic aci d	257.076 1	257.077 0			
					1.29	NEG	3.50
		Myrista					
959	C14H2 8O	ldehyd e	257.211 2	257.211 7			
					11.84	NEG	1.94
		(4R)-4- [(3R)-3- hydrox ybutyl]					
960	C13H2 2O2		228.195 6	228.195 7			
		-3,5,5-tr			8.29	POS	0.44

		imethyl cyclohe x-2-en- 1-one					
961	C14H2 9NO	Myrista mide	228.231 8	228.232 0		11.55 POS	0.88
		longitu					
962	C10H1 6N2O4	banine A	229.118 1	229.118 2		1.61 POS	0.44
963	C11H1 7NO3	mescali ne	229.154 5	229.154 6		3.45 POS	0.44
		N- acet yl-3-me thoxy-a					
964	C12H1 7NO2	mpheta mine	230.111 5	230.113 3		1.16 POS	7.82
		1,2-Ben zenedic arboxyl icacid, mono(2 -ethyl)					
965	C16H2 2O4	hexyles ter	259.133 4	259.133 4		10.04 NEG	0.00
966	C12H2 0O3	Garden one	230.174 3	230.174 7		9.22 POS	1.74
		ethyl a -D-fruc					
967	C8H16 O6	tofuran oside	231.083 7	231.083 8		1.23 POS	0.43
968	C13H1	(1R,3R)	231.112	231.112	4.36	POS	0.87

969	4N2O2	-1-meth yl-2,3,4, 9-tetrahydro-1 H-\$b-ca rboline- 3-carbo xylic a cid DECA NEDIO IC ACI D DIM	4	6			
	C12H2	ETHYL	231.158	231.158			
	2O4	ESTER (e)-2-he xenyl-b eta-d-gl	3	7	9.87	POS	1.73
970	C12H2	ucopyr	261.132	261.133			
	2O6	anoside 2,5,5-Tr imethyl -3-phen yl-cyclo	8	6	5.14	NEG	3.06
	C15H2	hexano	261.148	261.149			
971	0O	ne	4	0	10.21	NEG	2.30
	C15H2	Abscisi	263.127	263.128			
	0O4	c acid (6S)-2-	3	1	6.11	NEG	3.04
972	C15H2	methyl-	263.164	263.164			
	2O	6-[(1S)-	1	7	10.79	NEG	2.28
973	C15H2	methyl-	263.164	263.164			
	2O	6-[(1S)-	1	7	10.79	NEG	2.28

974		4-meth ylene-1 -cycloh ex-2-en yl]hept- 2-en-4- one gamma -l-gluta myl-l-b eta-ami noisibu					
	C9H16	tyric ac	233.112	233.112			
	N2O5	id	2	7	1.21	POS	2.14
975		2,2'biox azolidi ne-3,3'-					
	C10H2	diethan	233.149	233.149			
	0N2O4	ol	4	5	2.43	POS	0.43
976	C12H1	Cheria	236.091	236.091			
	3NO4	noine	7	7	2.15	POS	0.00
		3,7-dih ydroxy- 2,8-dim ethyl-9, 10-dihy drophe nanthre ne-4-ca					
977	C17H1	rbaldehy	267.101	267.102			
	6O3	de	5	1	7.92	NEG	2.25

		trans-1					
		0-Hept					
978		adecen					
	C17H3	oic aci	267.231	267.232			
	2O2	d	3	1	13.27	NEG	2.99
	C12H1	Secobar	239.138	239.138			
979	8N2O3	bital	5	7	5.82	POS	1.25
	C11H1	Wilford	241.117	241.117			
980	3NO4	ic acid	5	9	2.52	POS	1.66
	C15H2	artemis	269.211	269.211			
981	8O	inol	2	7	11.60	NEG	1.86
		3-Hydr					
982	C10H1	oxykyn	242.112	242.113			
	2N2O4	urenine	9	2	1.23	POS	1.24
		N-[2-(4-					
		Hydrox					
		ypheny					
983		l)ethyl]					
	C15H1	benzam	242.117	242.117			
	5NO2	ide	2	4	6.26	POS	0.83
		8-Deox					
984	C15H1	ylactuci	243.100	243.101			
	6O4	n	6	4	5.80	POS	3.29
		10-Hyd					
		roxy-3-					
		methox					
985		y-1,3,5,					
		7-cadin					
	C16H2	atetrae	243.137	243.137			
	0O3	n-9-one	2	9	7.97	POS	2.88
986	C11H1	pyrogl	271.093	271.093	1.60	NEG	0.00

	8N2O7	utamyl	0	0			
		glucos					
		amine					
		3-hydro					
987		xy-hexa					
	C16H3	decanoi	271.226	271.227			
	2O3	c acid	7	3	11.97	NEG	2.21
988	C16H3	Juniper	271.226	271.227			
	2O3	ic acid	7	3	10.72	NEG	2.21
989	C14H1	carbale	272.092	272.092			
	3NO2	xin a	0	4	6.15	NEG	1.47
990	C13H2	annuio	244.189	244.190			
	2O3	none e	9	3	7.14	POS	1.64
991	C15H1	Tectoq	245.060	245.059			
	0O2	uinone	9	1	3.91	POS	-7.35
		Glycyl-					
992	C11H1	pheny	245.089	245.089			
	4N2O3	lalanine	7	7	4.18	POS	0.00
		5-[(3aS,					
		6R,6aR)					
		-2-keto-					
		1,3,3a,4,					
		6,6a-he					
993		xahydr					
		othieno					
		[3,4-d]i					
		midazo					
	C10H1	l-6-yl]v					
	6N2O3	aleric a	245.094	245.094			
	S	cid	4	9	2.34	POS	2.04
994	C13H2	japonic	273.169	273.170	6.15	NEG	1.83

	4O3	umin	7	2			
		D					
		Cyclo(L					
995	C14H1	-Phe-L-	245.128	245.128			
	6N2O2	Pro)	0	2	5.12	POS	0.82
		5,9,13-P					
		entadec					
		atrien-2					
996		-one, 6,					
		10,14-tr					
	C18H3	imethyl	245.225	245.226			
	0O	-	6	3	12.13	POS	2.85
		γ-gluta					
997	C10H1	myl-val	247.128	247.128			
	8N2O5	ine	2	5	2.04	POS	1.21
		chinens					
998	C15H2	iolide	247.131	247.132			
	0O4	b	9	7	6.12	POS	3.24
		cyclo-					
999	C14H1	(phe-va	247.143	247.143			
	8N2O2	l)	3	7	2.17	POS	1.62
		3beta-H					
		ydroxy-					
1000	C15H2	atractyl	277.143	277.143			
	0O2	on	3	9	8.81	NEG	2.16
		2-PHE					
		NYLD					
1001	C18H3	ODEC	247.241	247.241			
	0	ANE	8	9	12.90	POS	0.40
	C11H2	2-c-met	279.108	279.108			
1002	2O9	hyl-d-e	0	0	2.11	NEG	0.00

		rythrito					
		l 1-o-β-					
		d-gluco					
		pyrano					
		side					
		Isorupe					
1003	C14H1	stonic	279.122	279.123			
	8O3	acid	4	1	7.65	NEG	2.51
1004	C13H1	xanthoc	249.075	249.075			
	2O5	erin	1	4	6.53	POS	1.20
		chelian					
1005	C12H9	sisamin	249.087	249.087			
	NO4	e	0	0	3.35	POS	0.00
		Senkyu					
1006	C12H1	nolide	249.109	249.109			
	8O4	N	1	4	6.51	POS	1.20
		methyl					
		guaia-					
1007		1(10),11					
		-dien-1					
	C16H2	5-carbo	249.184	249.184			
	4O2	xylate	3	6	11.03	POS	1.20
1008	C12H1	cnideol	281.065	281.066			
	2O5	B	5	1	6.07	NEG	2.13
1009	C11H2	jiogluti	250.164	250.164			
	0O5	n E	9	9	1.83	POS	0.00
		6,8-dih					
		ydroxy-					
1010		2-(2-ph					
	C17H1	enyleth	281.080	281.081			
	4O4	yl)chro	7	3	6.26	NEG	2.13

1011		mone					
		7-Hydr					
		oxy-2-					
1011		methyl-					
		4-oxo-4					
		H-1-be					
1011		nzopyr					
		an-5-ac					
	C12H1	etic aci	252.087	252.086			
1012	0O5	d	0	8	4.87	POS	-0.79
		regalosi					
	C12H1	de D_q	283.080	283.081			
1012	4O5	t	9	6	4.81	NEG	2.47
	C18H3	Isostear	283.262	283.263			
1013	6O2	ic acid	7	5	14.77	NEG	2.82
		6,7-def					
		ydroart					
1014	C15H2	emisini	255.132	255.134			
	0O2	c acid	5	0	3.51	POS	5.88
1015	C15H1	chrysar	285.075	285.076			
	2O3	obin	6	2	7.34	NEG	2.10
1016	C15H1	Mukoni	256.096	256.096			
	3NO3	ne	8	8	6.14	POS	0.00
1017	C16H1	omphal	256.132	256.132			
	7NO2	in	4	8	6.66	POS	1.56
		N-benz					
1018		oyl tyr					
		amine					
	C16H1	methyl	256.132	256.133			
1019	7NO2	ether	8	0	8.23	POS	0.78
	C14H2	n-ibdta	257.221	257.221	6.62	POS	2.72

1020	8N2O2		0	7			
		1,6-Dihydroxy-3,7-dimethoxyxanthone					
	C15H12O6		287.050	287.053			
1021		1,3-dihydroxy-4,5-dimethoxyxanthone					
	C15H12O6		287.054	287.055			
		2-methoxy-9,10-dihydrophenanthrene					
1022		e-4,5-diol					
	C15H14O3		287.091	287.091			
		D-gamma-glutamyl-D-glutamic acid					
1023							
	C10H16N2O7		259.093	259.093			
		d	0	0	1.20	POS	0.00
1024		saccharopine					
	C11H20N2O6		259.127	259.128			
		Diethyl					
1025		decanoate					
	C14H26O4		259.189	259.190			
			6	0	11.73	POS	1.54

1026	C9H18	lilioside	289.067	289.068	0.85	NEG	3.11
	O8	C	8	7			
1027		deacety			3.87	POS	0.77
		l asper					
1028	C11H1	acid_q	260.112	260.112	10.84	NEG	1.73
	4O6	t	5	7			
1029		9-aceto			7.41	NEG	0.35
		xythym					
1030	C17H2	ol 3-O-	289.143	289.144	8.32	POS	1.15
	2O4	tiglate	5	0			
1031		1-O-Ac			8.23	NEG	1.72
		etylbrit					
1032	C17H2	annilact	289.143	289.143	7.75	NEG	1.71
	4O5	one	8	9			
1033	C14H2	Isokob	261.124	261.124	4.77	POS	0.00
	2O2	usone	6	9			
1034	C15H1	Achilli	291.122	291.123	6.65	POS	1.52
	8O3	n	8	3			
1035		cryptol			5.48	POS	1.14
		epinon					
1036	C16H1	epinon	293.092	293.092	5.98	POS	1.90
	2N2O	e	2	7			
1037	C15H1	Jacquin	263.127	263.127	6.65	POS	1.52
	8O4	elin	8	8			
1038		shizuka			5.48	POS	1.14
		nolide					
1039	C15H1	Helenal	263.127	263.127	5.98	POS	1.90
	8O4	in	2	5			
1040	C15H1	chinens	263.126	263.127	5.98	POS	1.90
	8O4	iolide a	8	3			

1037	C14H1	gastrod	263.139	263.139			
	5NO3	amine	0	0	4.24	POS	0.00
1038	C15H2	Reynos	293.138	293.138			
	0O3	in	4	9	6.93	NEG	1.71
1039		11 β ,13-					
		dihydr					
1040	C15H2	o-3-epi	293.138	293.138			
	0O3	in c	4	9	7.42	NEG	1.71
1041		2-Phen					
		ylethyl					
1042	C16H2	octano	293.174	293.175			
	4O2	ate	8	3	9.29	NEG	1.71
1043	C17H2		293.211	293.211			
	8O	Sterol	2	7	11.12	NEG	1.71
1044	C17H1	hypode	265.133	265.133			
	3NO	matine	1	3	8.18	POS	0.75
1045		Feruloy					
	C14H2	lputres	265.154	265.154			
1046	0N2O3	cine	5	6	3.99	POS	0.38
		sodium					
1047		methy					
		lesculet					
1048	C12H1	in acet	295.044	295.045			
	0O6	ate	7	3	4.90	NEG	2.03
1049		2-hexyl					
	C16H3	decan-1	265.254	265.252			
1050	4O	-ol	4	3	12.90	POS	-7.92
		9-hydro					
1051	C18H3	xy-10,1	295.226	295.227			
	2O3	2-Octad	1	0	10.88	NEG	3.05

		ecadien					
		oic aci					
		d					
		9,10-Ep					
		oxy-12-					
1047		octadec					
	C18H3	enoic a	295.226	295.227			
	2O3	cid	3	1	11.57	NEG	2.71
	C17H3	Civeton	295.226	295.227			
1048	0O	e	2	1	11.92	NEG	2.71
		erythro					
		syringo					
		ylglyce					
1049		rol 8-O					
		-β-D-gl					
	C11H1	ucoside	267.087	267.085			
	6O6	_qt	9	9	6.55	POS	-7.49
		TRIBU					
		TYL P					
1050	C12H2	HOSP	267.171	267.171			
	7O4P	HATE	0	5	10.85	POS	1.87
		dofura					
1051	C14H1	nuronic	297.096	297.097			
	8O7	acid	4	2	4.88	NEG	2.69
		phenet					
1052	C18H1	hyl fer	297.111	297.112			
	8O4	ulate	6	4	9.03	NEG	2.69
		2,3-But					
		anediol					
1053	C10H2	glucos	297.117	297.118			
	0O7	ide	6	4	1.62	NEG	2.36

1054	C17H1	Asimilo	268.132	268.132			
	7NO2	bine	6	9	7.41	POS	1.12
1055	C17H1	(?)-caav	268.133	268.133			
	7NO2	erine	0	1	4.73	POS	0.37
1056		n-trans-cinnam					
	C17H1	oyltyra	268.132	268.132			
1057	7NO2	mine	6	9	7.29	POS	1.12
		1,5-di-isobutyl-3,3-dimethyl[3,1,0]-cyclohexadiene-4-Hydroxybenzoic acid					
1058	C16H2	lohexad	268.225	268.226			
	6O2	ione	7	4	9.95	POS	2.61
1059	C13H1	d gluc	299.076	299.076			
	6O8	oside	0	6	2.17	NEG	2.01
1060	C13H1	opuntio	299.076	299.076			
	8O9	side	5	6	3.80	NEG	0.33
1061		(+)-Lys					
	C16H1	ergic a	269.128	269.128			
1062	6N2O2	cid	4	4	4.57	POS	0.00
		Heptad					
1063	C17H3	ecan-2-	299.257	299.258			
	4O	one	8	5	13.12	NEG	2.34
1064	C16H1	alnusti	301.070	301.071			
	4O6	nol	3	0	6.81	NEG	2.33
1065	C17H1	2-Meth	301.106	301.107	8.97	NEG	2.99

	8O5	oxyben zyl-2,6- dimeth oxyben zoate	4	3			
1064	C8H9N O2	Metacet amol	301.117 7	301.118 6			
		1 beta, 4 beta, 7 alpha -trihydr			4.13	NEG	2.66
1065	C15H2 8O3	oxyeud csmene	301.200 5	301.201 3			
		4,8,12-t rimethy l-tridec			6.19	NEG	2.66
1066	C16H3 2O2	anoic a cid	301.237 0	301.237 7			
		16-Hex			9.99	NEG	2.32
1067	C16H3 0O2	adecan olide	272.257 6	272.258 0			
		9-Hexa decenoi			11.15	POS	1.47
1068	C16H3 0O2	c acid, (9Z)-	272.257 6	272.258 0			
		2,4,7-tri methox			7.96	POS	1.47
1069	C17H1 6O3	yphena nthrene	303.081 3	303.080 3			
					2.91	NEG	-3.30
1070	C15H1 8N2O4	p-Meth ylcinna	273.122 0	273.123 0			
					5.92	POS	3.66

1071		mic aci					
		d					
1072		11 β ,13-					
		dihydr					
	C15H2	oreynos	273.150	273.148			
	2O3	in	3	2	7.41	POS	-7.69
1073		3-meth					
		oxy-4-a					
1074		cetoxyc					
		innamy					
	C17H2	l angel	303.122	303.123			
	0O5	ate	4	1	8.51	NEG	2.31
1075		18-nord					
		ehydro					
1076		abietan					
	C19H2	-4alpha	273.220	273.220			
	8O	-ol	5	9	10.00	POS	1.46
1077		2-Hydr					
		oxypal					
	C16H3	mitic a	273.241	273.242			
	2O3	cid	8	1	12.39	POS	1.10
1078		(2R,3R,					
		4S)-2-(6					
1079		-amino					
		purin-9					
1080		-yl)-4-					
		(hydro					
1081		xymeth					
	C10H1	yl)oxol	274.091	274.091			
	3N5O3	an-3-ol	9	5	1.10	POS	-1.46
1082	C15H1	isoplaty	304.117	304.118	6.87	NEG	2.30

1077	7NO3	desmin e [(2S,3R, 4R,5R)- 5-(2,4-D ioxopyr imidin- 1-yl)-3, 4-dihyd roxyox olan-2- yl]meth yl dihy drogen	6	3			
	C9H13	phosp	305.016	305.017			
1078	N2O9P	hate 7-Meth oxy-5-p renylox	7	1	0.95	NEG	1.31
	C15H1	ycouma	305.101	305.102			
1079	6O4	rin gamma -l-gluta	7	4	9.33	NEG	2.29
	C10H1	myl-glu	276.117	276.118			
1080	7N3O6	tamine 1-unde cylenyl- 3,4-met hylene	6	3	0.90	POS	2.54
	C18H2	dioxyb	277.215	277.215			
	8O2	enzyme	6	9	7.37	POS	1.08

1081		(1(10)E, 2R,4R)- 2-meth oxy-8,1 2-epoxy germac ra-1(1 0),7,11-t rien-6-o					
	C16H2	ne(6),m	307.153	307.154			
	2O3	yr rhone	7	4	9.65	NEG	2.28
1082		Nona- 2,4-die noic ac	307.189	307.190			
	O2	id	9	7	8.54	NEG	2.60
		(2R,3S)- 2,3-dih ydroxy- 2-(4-hy droxyb enzyl)s					
1083	C11H1	uccinic	279.051	279.049			
	2O7	acid	7	6	5.96	POS	-7.53
		toxylox					
1084	C18H1	anthon	309.076	309.076			
	6O6	e c	3	3	8.38	NEG	0.00
		(3Z,6S,7 R)-3-bu tyliden					
1085	C16H2	e-6-but	279.159	279.159			
	2O4	ryrl-7-	1	1	9.02	POS	0.00

		hydrox					
		y-4,5,6,					
		7-tetrah					
		ydroiso					
		benzof					
		uran-1-					
		one					
		Glutam					
1086	C14H1	yltyrosi	309.108	309.108			
	8N2O6	ne	4	8	2.56	NEG	1.29
1087	C15H1	cocculo	279.170	279.170			
	9NO3	lidine	1	2	4.57	POS	0.36
1088	C15H2	teuclatr	279.192	279.192			
	8O3	iol	4	7	6.71	POS	1.43
		alpha-E					
1089	C18H3	leostear	279.231	279.231			
	0O2	ic acid	6	7	10.88	POS	0.36
1090	C9H18	Cerebr	311.107	311.108			
	N2O7	osid	8	7	0.79	NEG	2.89
1091	C15H1	rhinaca	281.077	281.078			
	4O4	nthin a	8	1	7.65	POS	1.07
1092	C18H3	tianshic	311.221	311.222			
	4O5	acid	8	0	8.77	NEG	0.64
		2-isopr					
		opyl-8-					
		methyl					
1093		phenan					
		threne-					
		3,4-dio					
	C18H1	ne(r0-0	282.148	282.148			
	6O2	90680)	1	5	7.80	POS	1.42

1094		METH					
		YL PA					
	C17H3	LMITO	313.236	313.237			
	2O2	LEATE	8	6	13.79	NEG	2.55
1095		L-Thre					
		o-Sphin					
	C18H3	gosine	282.277	282.278			
	7NO2	C-18	5	6	10.00	POS	3.90
1096		METH					
		YL 2-H					
		YDRO					
		XYOCT					
		ADEC					
	C19H3	ANOA	313.273	313.273			
	8O3	TE	0	9	13.04	NEG	2.87
1097	C15H2	Baptifol	283.137	283.139			
	0N2O2	ine	7	7	1.74	POS	7.06
		Benzoic					
1098		acid +					
	C13H1	2O, O	315.071	315.071			
	6O9	-Hex	1	6	2.83	NEG	1.59
1099	C20H3	coronar	315.195	315.195			
	0O4	in b	2	6	10.64	NEG	1.27
		L-2-Am					
1100		ino-4-m					
		ethylen					
		epenta					
	C6H9N	nedioic	317.097	317.098			
	O4	acid	0	0	1.47	NEG	3.15
1101	C16H2	clavatin	286.173	286.175			
	5NO2	e	7	7	3.97	POS	6.99

1102	C14H1	Swertia	319.044	319.045			
	0O6	nin	3	1	4.86	NEG	2.51
		imbrica					
1103	C20H3	taloic a	319.226	319.226			
	2O3	cid	0	9	11.07	NEG	3.13
		1'-Acet					
1104		oxyeug					
	C14H1	enol ac	287.093	287.091			
	6O5	etate	0	0	7.35	POS	-6.97
		2 α -hyd					
1105		roxyeu					
	C15H2	patolid	287.129	287.127			
	0O4	e	6	5	7.19	POS	-7.31
		7,10,13-					
		Hexade					
1106		catrien					
		oic aci					
		d, met					
1107	C17H2	hyl est	287.193	287.195			
	8O2	er	4	8	0.91	POS	8.36
1108	C11H1	Cardios	320.097	320.097			
	7NO7	permin	1	9	2.08	NEG	2.50
		m-digal					
1109	C14H1	loyl aci	321.023	321.024			
	0O9	d	2	2	4.19	NEG	3.12
		isoince					
1110	C20H3	nsole,o	321.241	321.242			
	4O3	xide	9	7	11.25	NEG	2.49
		5-[[(2S)-					
1110	C16H1	3,3-dim	289.102	289.105			
	6O5	ethylox	9	0	7.84	POS	7.26

		iran-2-y l]metho xy]-3,7- dihydr opyran o[3,2-f] benzof uran-2- one Meranz					
1111	C15H1 8O5	in hydr ate	323.113 0	323.113 3			
		Quinox alinedi one + 2Methy			7.46	NEG	0.93
1112	C15H2 0N2O6	l + C5 H11O4	323.123 4	323.124 1			
					4.47	NEG	2.17
1113	C16H1 8O5	aculeati n	291.122 2	291.122 5			
					9.14	POS	0.69
1114	C18H1 6O7	Cirsilin eol	325.071 4	325.071 3			
		6-O-ma lonyl-b eta-met hyl-D-g			7.42	NEG	-0.31
1115	C10H1 6O9	lucopyr anoside	325.075 8	325.076 7			
					0.92	NEG	2.77
1116	C16H1 8O4	Batatasi n II	292.153 3	292.153 8			
					8.32	POS	1.71
1117	C14H1	Boc-D-	326.123	326.123	2.37	NEG	1.84

	9NO5	Tyr-OH	3	9			
		polyace					
1118	C18H2	tylene	293.210	293.211			
	8O3	PQ-1	9	0	10.50	POS	0.34
		9-O-Me					
1119	C16H1	thylcou	327.045	327.048			
	0O5	mestrol	2	1	6.13	NEG	8.87
		15,16-bi					
		snor-13					
1120		-oxo-8					
		(17)-lab					
	C18H2	den-19-	293.210	293.211			
	8O3	oicacid	9	0	9.39	POS	0.34
		2,3-dim					
		ethoxy-					
1121		6-meth					
		yanthra					
	C17H1	quinon	327.092	327.089			
	4O4	e	4	9	6.47	NEG	-7.64
		cis-Pari					
1122	C18H2	naric a	294.241	294.242			
	8O2	cid	6	2	10.57	POS	2.04
		(4E,7E,					
		10Z,13					
		E,16E,1					
		9E)-Do					
1123		cosa-4,					
		7,10,13,					
		16,19-h					
	C22H3	exaenoi	327.230	327.231			
	2O2	c acid	9	9	12.95	NEG	3.06

	C10H1						
1124	2N5O6		328.043	328.044			
	P	CMP	1	2	1.18	NEG	3.35
		Ethyl,al					
1125		pha-hy					
	C16H3	droxym	295.228	295.226			
	2O3	yristate	4	4	7.37	POS	-6.77
		(1R,4S,6					
		R,8aR)-					
		1-(3-fur					
		yl)-4,6-					
		dihydr					
		oxy-5,8					
1126		a-dimet					
		hyl-4,6,					
		7,8-tetr					
		ahydro-					
		1H-isoc					
	C15H1	hromen	296.148	296.149			
	8O5	-3-one	7	0	5.80	POS	1.01
		lycojap					
1127	C17H2	onicum	296.166	296.164			
	3NO2	in C	1	1	9.65	POS	-6.75
		9,10,11-					
		Trihydr					
1128		oxyocta					
		dec-12-					
	C18H3	enoic a	329.232	329.232			
	4O5	cid	1	7	8.30	NEG	1.82
1129	C18H3	FA 18:	329.231	329.232			
	4O5	1+3O	9	6	8.11	NEG	2.13

1130		3''-meth					
		oxyasp					
	C18H1	arenydi	297.111	297.111			
	6O4	ol	3	7	4.37	POS	1.35
1131		isocryp					
	C19H2	totansh	297.147	297.148			
	0O3	i-none	5	0	7.57	POS	1.68
1132	C19H2	Helietti	297.147	297.148			
	2O4	n	3	2	9.69	POS	3.03
1133		(13S)-13					
		-hydro					
		xyoctad					
		eca-9,11					
	C18H3	-dienoi	297.241	297.242			
	2O3	c acid	6	0	10.02	POS	1.35
1134		beta-Gl					
	C13H1	ucogalli	331.065	331.066			
	6O10	n	5	3	2.35	NEG	2.42
1135		6-Gallo					
	C13H1	ylgluco	331.065	331.066			
	6O10	se	7	4	1.66	NEG	2.11
1136	C15H2	glurosi	331.141	331.140			
	4O8	de	0	4	3.87	NEG	-1.81
1137	C15H2	Panicul	298.163	298.164			
	0O5	ide B	9	4	6.65	POS	1.68
1138		Gibbere					
	C19H2	llin A6	331.153	331.154			
	4O5	1	5	3	6.93	NEG	2.42
1139		7,10-Oc					
	C18H3	tadecad	298.273	298.273			
	2O2	ienoic	0	5	8.72	POS	1.68

		acid					
		prelun					
1140	C15H1	ularicac	299.088	299.088			
	6O5	id	8	9	6.18	POS	0.33
		kaempferol-3-O- α -L-r					
1141	C15H1	hamnos	333.055	333.058			
	2O6	ide_qt	2	4	0.88	NEG	9.61
1142	C12H1		333.081	333.082			
	6O8	Phlorin	3	0	2.19	NEG	2.10
1143	C19H1		333.094	333.092			
	4N4	Bilin	6	9	1.25	NEG	-5.10
1144	C20H3	vaginat	333.205	333.206			
	0O4	in	3	2	9.81	NEG	2.70
		2-o-(3,4-dihydroxybenzoyl)-2,4,6-trihydroxyphenyl					
1145	C15H1	aceticac	303.047	303.049			
	2O8	id	7	1	4.35	POS	4.62
1146	C16H1	sappan	303.085	303.085			
	4O6	one b	1	7	5.22	POS	1.98
		protosa					
1147	C16H1	ppanin	303.086	303.086			
	4O6	c	3	3	4.80	POS	0.00
1148	C15H2	Des-O-	303.099	303.099			
	0O4	methyll	9	6	8.02	POS	-0.99

		asiodip					
		lodin					
1149	C20H3		303.230	303.231			
	0O2	Salviol	8	3	11.07	POS	1.65
1150	C14H1	isatan	338.086	338.087			
	5NO6	b	9	5	4.72	NEG	1.77
1151	C16H1	Vestito	304.115	304.116			
	4O5	ne	4	7	6.79	POS	4.27
1152	C13H1	Tricroz	339.033	339.034			
	0O8	arin A	6	7	1.80	NEG	3.24
1153	C16H1	casialac	305.101	305.101			
	6O6	tone	5	7	7.79	POS	0.98
		(S)-Tetr					
1154		ahydro					
	C20H2	columb	340.153	340.154			
	3NO4	amine	2	3	4.38	NEG	3.23
		3-(2-ket					
		o-3-met					
		hyl-but					
1155		-3-enyl)					
		-4,8-di					
		methox					
	C16H1	y-carbo	305.145	305.147			
	7NO4	styril	0	3	0.56	POS	7.54
		3,5-dim					
		ethoxy-					
1156		4-[(2S,3					
		R,4S,5S,					
		6R)-3,4,					
	C15H2	5-trihy	341.087	341.087			
	0O10	droxy-6	0	1	3.81	NEG	0.29

		-(hydro xymeth yl)oxan -2-yl]ox ybenzoi c acid Glucos					
1157	C15H2 0O10	yringic acid	341.086 2	341.086 7		NEG	
		1-hydro xy-2, 3, 5-trim ethoxyx			4.11		1.47
1158	C16H1 6O5	anthon e	306.132 7	306.133 2		POS	1.31
1159	C17H2 0O4	batatasi n v	306.168 8	306.169 4		POS	1.96
		Xantho sine (N ot vali					
1160	C10H1 2N4O6	dated)	307.063 5	307.064 2		POS	2.28
1161	C14H1 6O10	Theoga llin	343.064 9	343.066 0		NEG	3.21
	C10H1 2N5O7		344.037	344.039			
1162	P	PCG	8	0		NEG	3.49
		(E,E,E)- 3,7-11,1 6-tetra					
1163	C20H3 4O	methyl hexad	308.293 8	308.294 3		POS	1.62
					13.16		

		eca-2,6, 10,14-te traen-1- ol pipera					
1164	C18H2	mide c	346.164	346.165			
	3NO3	7:1(6 e)	4	2	8.07	NEG	2.31
		2,3,7-tri hydrox y-5-(3,4 -dihydr oxy-E-s tyryl)- 6,7,8,9-t etrahyd ro-5H-b enzocy					
1165	C19H2	clohept	311.126	311.127			
	0O5	ene	2	3	5.75	POS	3.54
		(3R)-7,2 '3'-Trih ydroxy- 4'-meth oxyisofl					
1166	C16H1	avanon	347.075	347.076			
	4O6	e	4	3	4.46	NEG	2.59
1167	C18H1	Ponga	312.128	312.125			
	4O4	mol	2	6	5.74	POS	-8.33
		1-(4-hy droxyb enzoyl)					
1168	C17H1	droxyb	313.117	313.118			
	3NO4	enzoyl)	7	0	5.88	POS	0.96

		-7-hydr oxy-6- methox yiso-qu inoline					
1169	C18H1 7NO3	oemero line	313.153 5	313.154 1		POS	1.92
		3-[4-(1 H-indol -3-yl)-3 H-thiaz ol-2-yl					
1170	C19H1 3N3S	dene]in dole	350.049 4	350.050 9		NEG	4.29
		(1R*,3R *,3'S*)- 1,2,3,4- Tetrahy dro-1- (2-thio- 3-pyrro lidinyl) -beta-ca rboline-					
1171	C16H1 7N3O2 S	3-carbo xylic a cid	350.070 1	350.071 8	1.17	NEG	4.86
		Senecio					
1172	C18H2 5NO6	nine N -oxide	350.158 9	350.159 9	5.06	NEG	2.86
1173	C17H1	Ladane	315.085	315.085	8.47	POS	1.59

1174	4O6	in	2	8			
		(12R)-1					
		2-Hydr					
1175		oxyocta					
		dec-9-e					
	C18H3	noic ac	316.283	316.284			
1176	4O3	id	6	1	11.01	POS	1.58
		Melilot					
	C17H1	ocarpa	317.101	317.101			
1177	6O6	n D	2	6	6.76	POS	1.26
		(+)-Har					
	C20H2	dwickii	317.205	317.208			
1178	8O3	c acid	7	4	11.19	POS	8.51
	C20H2	fibrauri	353.101	353.102			
	0O7	n	7	1	5.90	NEG	1.13
1179		9,10-di					
		hydrox					
	C18H3	ystearic	317.268	317.268			
1180	6O4	acid	0	3	10.46	POS	0.95
	C13H1	acalyph	318.119	318.118			
	9NO8	ine	1	7	1.24	POS	-1.26
1181		androst					
		ane-3,1					
	C19H3	1,17-tri	353.231	353.232			
1182	2O3	ol	5	4	7.39	NEG	2.55
	C19H2	miltipol	318.205	318.205			
	4O3	one	5	9	9.35	POS	1.57
1182		(3R,4S)-					
		3-(4-hy					
	C17H1	droxy-3	319.117	319.117			
	8O6	-metho	2	4	4.59	POS	0.63

		xy-benz					
		yl)chro					
		man-3,					
		4,7-triol					
1183	C10H1	cyclic	355.067	355.066			
	0N6O6	peptide	8	1	3.83	NEG	-4.79
		4-o-met					
1184		hyl epi					
	C17H1	sappan	319.116	319.116			
	8O6	ol	2	9	5.27	POS	2.19
1185	C20H2	melian	355.117	355.118			
	0O6	oninol	3	0	6.99	NEG	1.97
		cudrafl					
1186	C20H2	avanon	355.117	355.118			
	0O6	e b	3	0	9.22	NEG	1.97
		pseudo					
1187	C20H3	laricaci	319.225	319.226			
	0O3	d d	2	0	7.39	POS	2.51
		(2S,3S,4					
		R)-octa					
1188		decane-					
	C18H3	1,2,3,4-t	319.283	319.283			
	8O4	etrol	5	9	12.24	POS	1.25
		[3,4,5-tr					
		ihydrox					
		y-6-(hy					
1189		droxym					
		ethyl)o					
		xan-2-y					
	C14H1	l] 9-(hy	356.097	356.098			
	7NO7	droxym	3	0	2.10	NEG	1.97

		ethyl)-					
		2,2,6a,6					
		b,9,12a-					
		hexame					
		thyl-10-					
		[3,4,5-tr					
		ihydrox					
		y-6-[(3,					
		4,5-trih					
		ydroxy-					
		6-meth					
		yloxan-					
		2-yl)ox					
		ymethy					
		l]oxan-					
		2-yl]ox					
		y-1,3,4,					
		5,6,6a,7,					
		8,8a,10,					
		11,12,1					
		3,14b-te					
		tradeca					
		hydrop					
		icene-4					
		a-carbo					
		xylate					
		n-meth					
		yl tyra					
1190		mine-o-					
	C15H2	alpha-l-	320.141	320.144			
	3NO5	rhamno	9	4	0.92	POS	7.81

		pyrano					
		side					
		PSORO					
1191	C18H1	MIC A	357.059	357.060			
	4O8	CID	8	7	6.91	NEG	2.52
		przewa					
1192	C18H1	quinon	357.096	357.097			
	6O5	e f	5	2	7.53	NEG	2.24
		sulfoco					
1193	C15H2	stunoli	357.107	357.104			
	0O5S	de A	1	2	1.44	NEG	-8.12
		16α-hy					
		droxy-e					
1194		nt-kaur					
	C20H3	an-19-o	321.240	321.241			
	2O3	ic acid	4	4	10.66	POS	3.11
		(2Z)-2-					
		[(E)-3-c					
		yano-3-					
		[(2S,3R,					
		4S,5S,6					
		R)-3,4,5					
		-trihydr					
1195		oxy-6-					
		(hydro					
		xymeth					
		yl)oxan					
		-2-yl]ox					
		yprop-2					
	C14H1	-enylid	358.076	358.077			
	7NO10	ene]but	2	1	1.81	NEG	2.51

		anedioi					
		c acid					
1196	C18H2	coccutri	324.152	324.154			
	3NO3	ne	4	7	2.21	POS	7.10
1197	C17H2	sievers	324.179	324.179			
	2O5	n	3	9	5.82	POS	1.85
1198		3-Methoxytyramine-b					
	C18H2	etaxant	359.123	359.124			
	0N2O6	hin	2	0	4.74	NEG	2.23
1199		2-O-alpha-D-Galactopyranosyl-1-de					
	C12H2	oxynoji	326.143	326.144			
	3NO9	rimycin	4	0	0.85	POS	1.84
1200	C17H1	aristoliukine	327.096	327.097			
	1NO5	b	5	0	6.51	POS	1.53
1201		4-(4-Hydroxyphenyl)-2-butan					
	C16H2	one gl	327.147	327.145			
	2O7	ucoside	2	5	4.37	POS	-5.20
1202		threo-alpha-ustroba					
	C20H2	ilignan-	327.158	327.158			
	2O4	5	1	6	5.53	POS	1.53

1203		1-o-β-d -glucop yranos					
	C16H2	ylampl	361.148	361.149			
1204	6O9	exin	0	2	4.03	NEG	3.32
	C19H2	Artepill	361.159	361.162			
1205	4O4	in A	2	4	9.29	NEG	8.86
		Deacet					
1206	C20H2	yleupas	361.164	361.164			
	6O6	errin	0	8	6.69	NEG	2.22
1207		[(2R,5 R)-5-(2- Amino- 6-oxo-1 H-puri n-9-yl)- 3,4-dih ydroxy oxolan- 2-yl]me thyl di					
	C10H1	hydrog					
1208	4N5O8	en pho	362.049	362.049			
	P	sphate	1	9	1.44	NEG	2.21
1209	C20H2	leontici	328.189	328.190			
	5NO3	ne	9	3	5.57	POS	1.22
1210		8Z-eico					
	C20H3	senoic	328.319	328.320			
1211	8O2	acid	6	3	9.91	POS	2.13
	C18H1	cudrax	329.107	329.104			
1212	6O6	anthon	6	8	6.51	POS	-8.51

		e s					
1210	C19H2	Isotheb	329.186	329.186			
	1NO3	aine	2	1	4.94	POS	-0.30
1211	C18H2	fawcetti	330.202	330.203			
	9NO3	ine	3	1	4.31	POS	2.42
		4-hydro					
		xy-4-[2-					
		[(2R,3R,					
		4S,5S,6					
		R)-3,4,5					
		-trihydr					
		oxy-6-					
1212		(hydro					
		xymeth					
		yl)oxan					
		-2-yl]ox					
		yethyl]					
		cyclohe					
	C14H2	xan-1-o	365.143	365.144			
	4O8	ne	1	2	4.23	NEG	3.01
1213	C18H1	Samade	331.121	331.119			
	8O6	rin A	4	5	6.06	POS	-5.74
		paramil					
1214	C19H2	tioic ac	333.168	333.169			
	4O5	id	6	1	7.57	POS	1.50
1215	C19H2	Gibbere	334.199	334.200			
	4O4	llin A9	7	5	8.33	POS	2.39
		n-isobu					
		tyl-2 e,					
1216	C22H3	4 e,12z	334.309	334.309			
	9NO	-octade	1	8	13.54	POS	2.09

		catriena					
		mide					
		agarobi					
1217		ose di					
	C14H2	methyl	369.140	369.140			
	6O11	acetal	2	2	1.57	NEG	0.00
		wuling					
1218	C20H3	zhic ac	335.220	335.221			
	2O5	id	1	2	7.49	POS	3.28
		isopent					
1219	C15H2	enyalde	336.165	336.166			
	1N5O4	nosine	4	0	4.98	POS	1.78
		N-(2-M					
		ethylpr					
1220		opyl)oc					
		tadeca-					
	C22H4	2,4-die	336.325	336.325			
	1NO	namide	0	6	14.28	POS	1.49
		(z)-8-β-					
		d-gluco					
1221		pyrano					
		syloxic					
	C15H1	innami	371.096	371.097			
	8O8	cacid	2	3	4.66	NEG	2.96
		Tetrahy					
1222	C20H1	drocory	338.136	338.137			
	9NO4	samine	7	7	5.14	POS	2.96
1223	C16H2	thevesi	371.097	371.097			
	2O11	d	0	4	2.12	NEG	1.08
1224	C15H2	Indicin	338.152	338.154			
	5NO6	e-N-oxi	4	9	0.90	POS	7.39

		de					
1225	C21H2	(-)-Phill	371.148	371.149			
	4O6	ygenin	2	1	6.99	NEG	2.42
1226	C21H2	isoarcti	371.148	371.149			
	4O6	genin	0	0	7.16	NEG	2.69
		Dehydr					
1227	C20H1	ocreban	372.106	372.103			
	9NO4	ine	0	4	1.26	NEG	-6.99
		4-[(2S,3					
		R)-5-					
		[(E)-3-h					
		ydroxy					
		prop-1-					
		enyl]-7-					
		methox					
1228		y-3-met					
		hylol-2,					
		3-dihyd					
		robenz					
		ofuran-					
		2-yl]-2-					
		methox					
	C20H2	y-phen	341.136	341.137			
	2O6	ol	5	7	5.76	POS	3.52
1229	C20H3	isoince	341.266	341.267			
	6O4	nsolol	0	3	9.98	POS	3.81
		8-hydro					
1230		xy-10-h					
	C16H2	ydrosw	375.130	375.130			
	4O10	eroside	5	1	4.42	NEG	-1.07
1231	C19H1	methyl	343.116	343.117	5.91	POS	1.75

	8O6	ophio	4	0			
		pogona					
		none a					
1232	C19H2	diverso	377.158	377.159			
	4O5	side_qt	8	7	7.59	NEG	2.39
		6-Hydr					
		oxykae					
1233		mpferol					
		3,7,4'-t					
	C18H1	rimethy	345.095	345.096			
	6O7	l ether	3	1	5.21	POS	2.32
		(1r,2r)-					
		p-ment					
		h-4(5)-e					
		ne-1,2-					
1234		diol 1-					
		o-β-d-g					
		lu-copy					
	C16H2	ranosid	377.179	377.180			
	8O7	e	9	8	4.78	NEG	2.39
1235	C21H2	triptini	346.236	346.237			
	8O3	n a	3	0	10.99	POS	2.02
		Quercet					
		agetin					
1236		3,4'-di					
	C17H1	methyl	347.075	347.075			
	4O8	ether	1	6	7.20	POS	1.44
		9S,12R,					
		13R-tri					
1237	C18H3	hydrox	348.274	348.274			
	4O5	yoctade	0	2	7.37	POS	0.57

		c-10E-e noic ac id Prostag					
1238	C20H3	landin	381.221	381.225			
	2O4	B1	9	1	9.91	NEG	8.39
1239	C17H1	boeravi	351.047	351.047			
	2O7	none e	1	3	5.66	POS	0.57
1240	C18H3	Auxin	351.213	351.213			
	2O5	a	2	7	7.89	POS	1.42
1241	C20H3	leohete	352.245	352.247			
	0O4	rin	8	0	9.16	POS	3.41
		Sieges methyl					
1242	C21H3	etheric	352.283	352.283			
	4O3	acid	0	8	12.03	POS	2.27
		6,7,10-T rihydro xy-8-oc tadecen					
1243	C18H3	oic aci	353.229	353.229			
	4O5	d	2	5	8.10	POS	0.85
1244	C20H1	Daphne	385.091	385.092			
	8O8	ticin	1	0	6.13	NEG	2.34
1245	C20H1	angusto	354.115	354.118			
	7N3O2	line	1	2	4.05	POS	8.75
		daurip					
1246	C19H1	orphin	355.128	355.128			
	5NO5	oline	2	5	4.57	POS	0.84
1247	C22H4	11-doco	356.351	356.351			
	2O2	senoic	1	7	12.70	POS	1.68

		acid					
	C19H2						
1248	0N2O3	Pioglitazone	357.129	357.128			
	S	methylester	5	1	1.24	POS	-3.92
1249		6-o-p-cis-coumaroyl-β-d-glucopyranoside					
	C16H20O8	7-Hydroxy-5,6,8,4'-tetramethoxy-5,6,7,4'-tetrahydroxykaempferol	358.148	358.149			
			6	1	4.44	POS	1.40
1250							
	C19H18O7	6-Hydroxykaempferol-3,6,7,4'-tetramethylether	359.109	359.111			
			7	1	7.53	POS	3.90
1251							
	C19H18O7	ethyl ether	359.111	359.112			
			7	1	9.84	POS	1.11
1252		Argininosyl-glucose					
	C12H24N4O7	qt	359.153	359.153			
			1	4	0.76	POS	0.84
1253	C20H23NO4	(+)-Thaliporph	359.195	359.195			
			3	9	5.40	POS	1.67

		ine					
1254	C22H3	caesalpi	359.219	359.221			
	2O5	nin k	7	0	8.19	POS	3.62
		homost					
1255	C20H2	ephano	360.178	360.179			
	5NO5	line	9	7	4.37	POS	2.22
		14-deox					
		y-11-ox					
1256		a-andro					
	C20H2	graphol	393.197	393.194			
	8O5	ide	1	5	6.43	NEG	-6.61
1257	C19H2	typhic	361.127	361.127			
	0O7	acid	6	9	7.57	POS	0.83
		(2S,3R,4					
		S,5S,6					
		R)-2-[4-					
		(2-hydr					
		oxyeth					
		yl)-2,6-					
		dimeth					
1258		oxy-ph					
		enoxy]-					
		6-meth					
		ylol-tet					
		rahydr					
		opyran-					
	C16H2	3,4,5-tri	361.145	361.147			
	4O9	ol	1	2	3.71	POS	5.81
		[(3S,8S,					
1259	C23H3	9S,10R,	361.272	361.272			
	6O3	13S,14	1	9	10.39	POS	2.21

		S,17S)-1					
		7-(1-hy					
		droxyet					
		hyl)-10,					
		13-dim					
		ethyl-2,					
		3,4,7,8,					
		9,11,12,					
		14,15,1					
		6,17-do					
		decahy					
		dro-1H					
		-cyclop					
		enta[a]					
		phenan					
		thren-3-					
		yl] acet					
		ate					
1260	C14H1	vulgaxa	362.096	362.096			
	7N3O7	nthin i	5	2	0.84	POS	-0.83
		beta-ap					
1261		opicrop					
	C22H2	odophy	395.111	395.112			
	0O7	llin	6	6	9.13	NEG	2.53
1262	C20H3	dictam	397.184	397.185			
	2O9	noside,l	9	5	4.64	NEG	1.76
1263	C24H3	gancao	397.199	397.201			
	0O5	nin T	9	0	10.73	NEG	2.77
		27-nor-					
1264	C27H4	(24R)-	367.334	367.335			
	4O	methyl	1	3	14.39	POS	3.27

		cholest-					
		5,22E-d					
		ien-3be					
		ta-ol					
		carboxy					
1265	C20H1	evodia	370.109	370.112			
	7N3O3	mine	0	6	2.71	POS	9.73
1266	C14H2	koabur	371.073	371.073			
	0O9	aside	1	5	3.10	POS	1.08
		Diethyl					
1267	C22H4	hexyl a	371.314	371.315			
	2O4	dipate	4	0	14.99	POS	1.62
		methyl					
		(1R,4a					
		S,7R,7a					
		S)-4a,7-					
		dihydr					
		oxy-7-					
		methyl-					
1268		1-[(2S,3					
		R,4S,5S,					
		6R)-3,4,					
		5-trihy					
		droxy-6					
		-(hydro					
		xymeth					
		yl)oxan					
		-2-yl]ox					
		y-1,5,6,					
	C17H2	7a-tetra	405.138	405.139			
	6O11	hydroc	2	2	1.96	NEG	2.47

		yclopen ta[d]py ran-4-c arboxyl ate					
1269	C16H2 6O9	Villosol side	407.154 3	407.155 1			
		(3s,6r)- 6,7-dih ydroxy- 6,7-dih ydrolin alool-3- o-β-d-g			3.74	NEG	1.96
1270							
	C16H3 0O8	lucopyr anoside	373.182 8	373.183 0			
					4.16	POS	0.80
1271	C11H1 2N2O2	pegami ne	407.169 6	407.171 0			
					3.75	NEG	3.68
1272	C21H3 0O5	postster one	407.205 9	407.206 7			
					5.63	NEG	1.96
		2-[(9Z,1 2Z)-hep tadeca- 9,12-die nyl]-6-h ydroxy					
1273							
	C24H3 6O3	benzoic acid	373.273 1	373.273 4			
					8.97	POS	0.80
1274	C24H2 8O6	pongap inone b	411.179 5	411.180 4			
					8.19	NEG	2.19
1275	C18H2	celepht	413.143	413.144	4.96	NEG	1.94

	4O8	alide a	7	5			
1276	C22H2	Sphaer	413.158	413.159			
	4O5	osinin	3	4	6.62	NEG	2.90
		14-deox					
		y-12(R)					
1277		-sulfoa					
		ndrogr					
	C20H3	apholid	413.167	413.165			
	0O7S	e	3	6	3.69	NEG	-4.11
		Isoprop					
1278		yl apio					
	C14H2	sylgluc	377.141	377.141			
	6O10	oside	0	4	2.16	POS	1.06
		XYLOS					
1279	C18H2	TOSIDI	414.128	414.125			
	5NO8S	NE	2	5	1.44	NEG	-6.52
1280	C22H2	Elegani	415.138	415.138			
	6O9	n	5	9	7.30	NEG	0.96
		cynatra					
1281	C21H2	toside	378.225	378.226			
	8O5	B_qt	5	5	7.58	POS	2.64
		Kaempferol 7-					
1282							
	C20H1	arabino	417.081	417.081			
	8O10	side	1	9	6.17	NEG	1.92
		2,3-dih					
1283	C18H1	ydroiri	380.133	380.133			
	8O8	genin	0	5	3.81	POS	1.32
1284	C24H2	Chloro	381.205	381.205			
	8O4	phorin	4	7	10.33	POS	0.79
1285	C20H1	12a-Hy	383.075	383.075	6.35	POS	1.04

	4O8	droxyp achyrrh izone Senkyu	3	7			
1286	C24H3 0O4	nolide- P	383.220 9	383.221 3			
		p-hydr oxyben zoyl ca			11.15	POS	1.04
1287	C20H2 2O10	lleryani n	421.111 2	421.112 6			
		Adoxos			4.56	NEG	3.32
1288	C16H2 4O10	idic aci d	421.133 5	421.134 3			
					1.69	NEG	1.90
1289	C18H2 5NO7	Spectab iline	385.195 1	385.196 0			
		STICTI			1.32	POS	2.34
1290	C19H1 4O9	C ACI D	387.071 0	387.071 0			
					4.33	POS	0.00
1291	C21H1 6O6	Gerberi nol	387.083 1	387.083 5			
		inumak			9.41	POS	1.03
1292	C18H2 0O8	ilactone a	387.108 2	387.106 6			
		(2S,3S,4 R,5R,6 R)-3-[(2 S,3R,5S, 6R)-3-a			5.22	POS	-4.13
1293	C14H2 3NO11	cetamid o-5-hyd	426.126 9	426.126 1			
					1.66	NEG	-1.88

		roxy-6-					
		(hydro					
		xymeth					
		yl)oxan					
		-2-yl]ox					
		y-4,5,6-					
		trihydr					
		oxyoxa					
		ne-2-ca					
		rboxyli					
		c acid					
		dehydr					
1294	C17H2	ologani	389.138	389.141			
	4O10	n	6	4	4.22	POS	7.20
		(2S)-6-					
		(2,4-dih					
		ydroxy					
		phenyl)					
		-2-(2-hy					
		droxyp					
		ropan-2					
1295		-yl)-4-					
		methox					
		y-2,3-di					
		hydrof					
		uro[3,2-					
		g]chro					
	C21H2	men-7-	429.117	429.118			
	0O7	one	1	1	5.86	NEG	2.33
1296	C20H3	androg	429.161	429.160			
	0O8S	rapholi	9	4	2.06	NEG	-3.50

		de-3-o-sulfate					
		Dioctyl					
1297	C24H3	phthal	391.282	391.283			
	8O4	ate	9	6	14.97	POS	1.79
1298	C18H2	scelerat	392.163	392.165			
	7NO7	ine	8	9	1.18	POS	5.35
		16-Prop					
1299	C24H2	oxystry	393.221	393.219			
	8N2O3	chnine	5	4	13.61	POS	-5.34
1300	C17H2	majoros	433.133	433.134			
	4O10	ide	1	1	4.08	NEG	2.31
1301	C24H4	pallaso	394.330	394.331			
	0O3	ne b	4	0	14.25	POS	1.52
1302	C20H2	stephas	395.215	395.216			
	7NO6	unoline	3	5	4.05	POS	3.04
		acetic a					
		cid [(1					
		R,3R,4					
		R,4aS,8					
		aS)-4-h					
		ydroxy-					
		4-[2-(2-					
1303		keto-3-					
		pyrroli					
		n-3-yl)e					
		thyl]-3,					
		4a,8,8-t					
		etramet					
	C22H3	hyl-dec	395.289	395.289			
	5NO4	alin-1-y	2	8	13.86	POS	1.52

1304		l] ester					
		3-[[[(2S)-					
		2,4-Dih					
		ydroxy-					
		3,3-dim					
		ethylbu					
		tanoyl]					
		amino]					
		propan					
	C9H17	oic aci	437.211	437.212			
	NO5	d	5	8	2.90	NEG	2.97
1305	C24H2	Gancao	398.231	398.231			
	8O4	nin U	2	9	12.59	POS	1.76
1306	C21H1	Prostali	439.060	439.063			
	4O8	din A	3	7	6.33	NEG	7.74
1307	C24H2	Confer	398.232	398.232			
	8O4	one	0	3	11.00	POS	0.75
1308		(e)-2-he					
		xenyl-α					
		-l-arabi					
		nopyra					
		nosyl-					
		(1→2)-					
		β-d-glu					
	C17H3	copyra	439.178	439.180			
	0O10	noside	5	3	4.35	NEG	4.10
1309		(3E,4R)-					
		4-(1,3-b					
		enzodi					
	C22H2	oxol-5-	399.143	399.143			
	2O7	ylmeth	1	4	9.43	POS	1.00

		yl)-3- [(3,4,5-t rimetho xyphen yl)meth yliden e]oxola n-2-one					
1310	C22H3 2O5	galeops in	399.209 6	399.211 9		1.49 POS	5.76
1311	C22H3 2O5	prehu mulone	399.218 8	399.216 5		10.33 POS	-5.76
1312		Phthali c acid, isobut yl und					
	C23H3 6O4	ecyl est er	399.249 8	399.250 2		11.24 POS	1.00
1313		beta-Sit osterol- beta-D- glucop					
	C27H4 2O2	yransosi de_qt	399.326 7	399.326 2		10.00 POS	-1.25
1314		(2S,3S)- pteros in C 3- O- β- glucop					
	C20H2 8O8	yransosi de	441.174 8	441.175 7		5.51 NEG	2.04

1315	C20H3	masson	443.190	443.191			
	0O8	ivesinol	1	2	4.03	NEG	2.48
1316	C27H4		401.341	401.341			
	4O2	abricin	6	5	8.94	POS	-0.25
1317	C18H2	Acetylc	447.148	447.149			
	6O10	atalpol	4	6	4.37	NEG	2.68
1318	C27H4	δ-tocop	447.353	447.350			
	6O2	herol	8	9	9.99	NEG	-6.48
1319		staphyl					
	C20H3	ionosid	403.233	403.233			
1320	6O9	e i	6	4	4.73	POS	-0.50
		(8S,9S,1 0R,13R, 14S,17 R)-10,1 3-dimet hyl-17- [(E,1R,4 R)-1,4,5 -trimet hylhex- 2-enyl]- 2,3,8,9,1 1,12,14, 15,16,17 -decahy dro-1H -cyclop enta[a]					
	C28H4	phenan	403.337	403.335			
	4	threne	1	3	7.27	POS	-4.46

1321		1,3-dihydroxy-4,5-dimethoxyxanthone-3-o-beta-d-glucopyranoside	449.108	449.108			
	2O11		1	5	4.62	NEG	0.89
1322	C22H2	Prupersin	449.143	449.144			
	6O10		3	3	4.68	NEG	2.23
1323	C19H3	ionoside	449.201	449.202			
	2O9	e c ethyl c	2	0	4.80	NEG	1.78
1324	C18H2	hlorogenate	405.118	405.117			
	2O9		8	2	5.23	POS	-3.95
1325	C23H3	corotoxin	406.258	406.258			
	2O5	igenin 3-Hydr	4	6	7.57	POS	0.49
1326	C25H2	oxyglabrol	453.190	453.191			
	8O5	Ceanothenic acid	1	0	10.17	NEG	1.99
1327	C29H4	henic acid	453.298	453.299			
	2O4	24-Dehydrocholesterol	4	7	11.56	NEG	2.87
1328	C27H4	olesterol	407.332	407.330			
	4O		6	5	8.51	POS	-5.16
1329	C23H2	10-methoxy-20	455.100	455.101			
	0N2O6		9	2	0.77	NEG	0.66

		-o-acety lcampt othecin					
1330	C23H2 0O7	rhinaca nthin d	409.126 8	409.127 5			
		(2S,3S)- pteros in S- 1			6.96	POS	1.71
1331		4- O- β -glucop					
	C20H2 8O9	yransosi de	457.169 7	457.170 6			
					5.06	NEG	1.97
1332	C17H3 2O11	Grando side	457.191 1	457.191 9			
					3.83	NEG	1.75
1333	C22H2 0O11	Palustri noside	459.092 1	459.092 7			
		3-[3-[5- (2-carb oxyeth yl)-2-hy droxy-3 -metho xyphen yl]-4-hy droxy-5 -metho xyphen yl]prop					
1334	C20H2 2O8	anoic a cid	413.123 5	413.122 1			
					5.21	POS	-3.39
1335	C17H2	harpagi	413.140	413.140	3.96	POS	2.18

	6O10	de acet 0	9				
		ate					
		2,3-Deh					
1336		ydrosil					
	C25H2	ychristi	461.083	461.085			
	0O10	n	4	3	6.28	NEG	4.12
1337	C19H2	Sayaen	461.164	461.165			
	8O10	doside	1	3	4.46	NEG	2.39
1338	C23H2	cniforin	415.174	415.174			
	6O7	B	5	8	10.81	POS	0.72
		pseudo					
1339		protodi					
	C27H4	oscin_q	415.319	415.320			
	2O3	t	2	0	9.03	POS	1.69
		STOCK					
1340	C27H4	1N-663	415.319	415.320			
	2O3	70	7	2	7.89	POS	1.20
1341	C24H3	assafoet	416.242	416.242			
	0O5	idnol a	5	8	10.31	POS	0.72
1342	C25H2	Kuwan	465.151	465.153			
	4O6	on B	7	6	6.93	NEG	4.08
1343	C26H2	Kanzon	465.185	465.188			
	8O5	ol F	0	4	10.32	NEG	7.52
		3alpha,					
		7alpha-					
		Dihydr					
1344		oxy-5be					
		ta-chole					
		stan-26-					
	C27H4	oic aci	417.334	417.335			
	6O4	d	9	9	11.18	POS	2.40

1345		24, 25- Dihydr					
	C27H4	oxy V	417.335	417.335			
	4O3	D3	5	9	9.63	POS	0.96
1346		pterosi n c-3-o					
	C20H2	-glucosi	419.171	419.169			
	8O8	de	4	5	6.29	POS	-4.53
1347		scutba rbatine					
	C26H3		470.216	470.217			
	3NO7	K	6	5	10.33	NEG	1.91
1348		Benzyl alcohol					
	C18H2	+ Hex	420.184	420.185			
	6O10	-Pen	2	3	4.37	POS	2.62
1349		Picraqu assiosid					
	C18H2		421.109	421.110			
	2O10	e A	9	2	4.99	POS	0.71
1350		3,4-tera crylshi					
	C23H2		421.156	421.159			
	6O6	konin	8	5	2.41	POS	6.41
1351		24-Met hylchol esta-7,2 2-dien-					
	C28H4	3beta-o	421.347	421.345			
	6O	l	5	8	7.27	POS	-4.03
1352		pirolati n					
	C23H3		473.197	473.196			
	4O8		2	0	7.90	NEG	-2.54
1353		Marcha ntin A					
	C28H2		475.126	475.129			
	4O5		2	0	0.94	NEG	5.89

		Phenet					
1354	C20H3	hyl rut	475.179	475.181			
	0O10	inoside	9	0	4.76	NEG	2.31
1355	C17H2	Lamiid	423.147	423.148			
	6O12	e	5	6	3.64	POS	2.60
1356	C24H3	karatav	423.214	423.214			
	2O5	icin	0	1	10.55	POS	0.24
1357	C21H2	Sulfurei	477.101	477.102			
	0O10	n	7	8	4.52	NEG	2.31
		Isorha					
1358		mnetin					
	C22H2	3-gala	477.101	477.102			
	2O12	ctoside	5	7	4.70	NEG	2.52
1359	C22H2	Homon	477.149	477.144			
	4O9	ataloin	2	7	0.82	NEG	-9.43
		4-hydro					
		xyphen					
1360		yl-β-ge					
	C18H2	ntiobio	479.139	479.139			
	6O12	side	0	8	2.63	NEG	1.67
		alpha-					
1361	C30H4	Amyro	425.379	425.378			
	8O	ne	0	4	12.98	POS	-1.41
		Malloto					
1362	C21H2	phenon	427.139	427.138			
	4O8	e	9	1	6.55	POS	-4.21
		Gallic					
		acid 3-					
1363		O-(6-ga					
	C20H2	lloylglu	483.076	483.077			
	0O14	coside)	8	4	4.26	NEG	1.24

1364	C25H2	Morusi	483.164	483.165			
	6O7	gnin L	0	0	8.81	NEG	2.07
		Ponga					
1365	C23H2	moside	485.102	485.105			
	0O9	A	3	6	4.88	NEG	6.80
		akebon					
1366	C29H4	oic aci	485.325	485.326			
	4O3	d	4	3	11.47	NEG	1.85
		5beta-C					
		holesta					
		ne-3alp					
1367		ha,7alp					
		ha,12al					
		pha,26,					
	C27H4	27-pent	487.321	487.320			
	8O5	ol	1	4	8.96	NEG	-1.64
1368	C21H2	glaucog	431.148	431.147			
	8O7	enin b	7	7	3.85	POS	-2.32
1369	C22H1	nyssosi	489.060	489.064			
	8O13	de	7	1	4.34	NEG	6.95
1370	C27H4	isonuat	431.315	431.315			
	2O4	igentin	0	3	6.39	POS	0.70
1371	C26H3	taxuspi	489.213	489.213			
	6O10	ne o	7	1	7.49	NEG	-1.23
		tyramin					
1372	C27H2	oporph	491.141	491.139			
	4N2O5	ine	1	5	4.16	NEG	-3.26
1373	C19H2	Bungei	491.138	491.139			
	6O12	side D	8	7	3.88	NEG	1.83
1374	C22H2	isosaku	433.148	433.148			
	4O9	ranetin-	3	8	6.02	POS	1.15

1375		7-rutin oside (Z)-(1S, 5R)-bet a-pinen -10-yl-b					
	C21H3	eta-vici	491.211	491.212			
	4O10	anoside (1s,4s,5 s,7r,10 r)-10,1 1,14-tri hydrox yguai-3 -one 11 -o-β-d- glucop	8	6	5.80	NEG	1.63
1376							
	C21H3	yransi	433.244	433.243			
	6O9	de 3-O-me thylella gic aci d-4'-O- β-D-xyl	4	8	4.91	POS	-1.38
1377							
	C20H1	opyrosi	493.060	493.061			
	6O12	de 1-(beta- carboli n-1-yl)-	6	5	3.74	NEG	1.83
1378							
	C29H2	4-(4,8-d	493.183	493.185			
	6N4O4	imetho	7	9	7.88	NEG	4.46

1379		xy-beta					
		-carboli					
		n-1-yl)-					
		2-meth					
		oxy-but					
		an-1-on					
		e					
		[7-(2-m					
		ethylbu					
		t-2-eno					
1380		yloxy)-					
		4-oxido					
		-5,6,7,8-					
		tetrahy					
		dro-3H					
		-pyrroli					
		zin-4-iu					
		m-1-yl]					
		methyl					
		2,3-di					
1380		hydrox					
		y-2-(1-h					
		ydroxy					
		ethyl)-3					
		-methyl					
	C20H3	butano	436.188	436.191			
	1NO8	ate	8	5	1.37	POS	6.19
		butyl 3					
		-[3-met					
	C20H3	hoxy-4-	437.181	437.179			
1380	0O9	[(2S,3R,	6	9	5.21	POS	-3.89

1381

4S,5S,6
R)-3,4,5
-trihydr
oxy-6-
(hydro
xymeth
yl)oxan
-2-yl]ox
ypheny
l]propa
noate
(2S,3S)-
3,5-dih
ydroxy-
2-(4-hy
droxyp
henyl)-
8-(3-me
thylbut
-2-enyl)
-7-[(2S,
3R,4S,5
S,6R)-3,
4,5-trih
ydroxy-
6-meth
ylol-tet
rahydr
opyran-

C26H3	2-yl]ox	499.159	499.160			
0O11	y-chro	6	0	6.08	NEG	0.80

1382		man-4-					
		one					
		1,6-bis					
		(4-hydr					
		oxyben					
		zyl)-4-					
		methox					
		y-9,10-					
		di-hydr					
		ophena					
		nthrene					
	C29H2	-2,7-dio	499.178	499.177			
	6O5	l	4	3	2.12	NEG	-2.20
		Pentah					
1383		ydroxy					
	C28H5	bufosta	501.336	501.335			
	0O5	ne	1	6	8.97	NEG	-0.80
1384	C23H3	(-)-gom	441.169	441.168			
	0O6	isin k1	4	4	5.88	POS	-2.27
		Soyasa					
1385	C30H4	pogeno	441.372	441.372			
	8O2	l C	3	5	7.37	POS	0.45
1386	C23H2	Icarisid	507.159	507.155			
	6O10	e A7	6	2	0.83	NEG	-8.68
1387	C26H3	kushen	507.178	507.178			
	2O8	ol h	7	9	8.12	NEG	0.39
1388	C22H2	(±)-lyon	443.167	443.167			
	8O8	iresinol	2	4	6.18	POS	0.45
		8-o-(2-h					
1389	C24H3	ydroxy	509.163	509.165			
	0O12	cinnam	9	1	5.36	NEG	2.55

		oyl)har					
		pagide					
		Androg					
1390	C23H2	raphidi	445.147	445.148			
	6O10	n A	3	6	6.54	POS	2.92
		p-β-ruti					
1391		nosylox					
	C20H2	y styre	446.202	446.202			
	8O10	ne	3	2	4.75	POS	-0.22
		Neosily					
1392	C25H2	hermin	511.133	511.129			
	2O9	A	8	2	1.82	NEG	-9.00
		agrimo					
		nolide-					
1393		6-o-β-d					
		-glucop					
	C24H2	yransosi	511.139	511.138			
	8O10	de	3	4	6.02	NEG	-1.57
1394	C23H3	pikuros	511.143	511.144			
	0O14	ide	6	4	4.18	NEG	1.57
1395	C26H2	Jangom	513.174	513.175			
	8O8	olide	6	6	9.15	NEG	1.95
		2,3,5,4'-					
		tetrahy					
		droxyst					
		ilbene-2					
1396		-o-(6''-o					
		-acetyl)					
		-beta-d-					
	C22H2	glucop	449.143	449.143			
	4O10	yransosi	0	6	5.21	POS	1.34

		de					
		Isochlo					
1397	C25H2	rogenic	515.116	515.118			
	4O12	acid b	7	1	4.48	NEG	2.72
		11-oxo-					
1398	C30H4	kansen	515.338	515.338			
	6O4	onol	6	2	9.99	NEG	-0.78
1399	C24H3	piperka	453.187	453.187			
	0O7	dsin B	4	9	10.16	POS	1.10
		(2R,3					
		R)-6 [1-					
		(4'-hydr					
		oxy-3'-					
		methox					
1400		ypheny					
		l)prop-					
		2en-1-y					
		1] -pino					
		banksin					
	C27H2	-3-aceta	521.143	521.144			
	4O8	te	1	2	7.20	NEG	2.11
		luciden					
1401	C27H4	ic acid	521.273	521.274			
	0O7	O	4	5	5.98	NEG	2.11
		saikosa					
1402	C30H4	ponin	455.350	455.351			
	8O4	b1_qt	0	3	9.51	POS	2.85
		3β-hyd					
1403		roxylan					
	C30H4	osta-7,9	455.350	455.351			
	6O3	(11),24-	8	4	7.12	POS	1.32

		trien-21					
		-oic aci					
		d					
		hespere					
		tin-7-O-					
1404		β-D-glu					
	C22H2	curonid	523.107	523.108			
	2O12	e	1	2	4.10	NEG	2.10
	C22H2	ciwujiat	457.145	457.146			
1405	6O9	one	5	2	5.52	POS	1.53
		2,3-Deh					
1406	C25H2	ydrosil	525.112	525.108			
	0O10	ybin	8	3	0.92	NEG	-8.57
	C27H3	Wusha	529.168	529.170			
1407	0O11	nicariin	9	2	6.06	NEG	2.46
	C28H2	isoricca	463.129	463.130			
1408	4O4	rdin c	8	2	12.45	POS	0.86
	C21H2	Cichori	463.156	463.156			
1409	8O10	oside B	3	9	5.15	POS	1.30
	C26H3	kihada	531.185	531.186			
1410	0O9	nin b	1	1	8.02	NEG	2.07
		18alpha					
		-Hydro					
1411		xyglycy					
	C30H4	rrhetic	531.331	531.331			
	6O5	acid	0	9	10.45	NEG	1.51
		(z)-(1s,5					
		r)-beta-					
1412		pinen-1					
	C21H3	-oxy-be	464.248	464.248			
	4O10	ta-vicia	0	5	5.79	POS	1.08

		noside					
		polyca					
1413	C26H3	udosid	533.164	533.165			
	0O12	e a	4	4	4.94	NEG	1.88
1414	C26H3	Phellati	533.175	533.170			
	0O12	n	4	9	0.85	NEG	-8.44
		berche					
		mol-4'-					
1415		o-β-d-g					
	C26H3	lucosid	537.195	537.196			
	4O12	e	8	8	4.52	NEG	1.86
1416	C31H3	taxezop	537.250	537.250			
	8O8	idin e	8	1	8.97	NEG	-1.30
1417	C18H3		539.136	539.137			
	2O16	Panose	8	6	1.30	NEG	1.48
		Diosge					
1418	C29H4	nin ace	474.356	474.357			
	4O4	tate	4	1	9.02	POS	1.48
1419	C28H2	rhinaca	475.177	475.176			
	6O7	nthin q	1	1	0.90	POS	-2.10
1420	C26H3	Ensacul	475.214	475.217			
	2N2O5	in	7	5	4.49	POS	5.89
1421	C26H3	graucin	547.180	547.181			
	0O10	a	6	3	5.60	NEG	1.46
		6-O-p-c					
1422		oumaro					
	C24H3	ylajugo	477.170	477.173			
	0O11	l	7	4	5.21	POS	5.66
1423	C24H4	cuneata	549.254	549.255			
	0O11	side e	8	0	5.10	NEG	0.36
1424	C25H3	tenuiph	551.139	551.139	4.08	NEG	0.73

	0O15	enone b	3	7			
1425	C30H2	Rheidin	553.119	553.116			
	0O8	B	0	5	4.28	NEG	-4.52
1426	C21H3		481.171	481.169			
	0O11	Gein	2	6	5.27	POS	-3.33
		Arginin					
1427	C18H3	yl-fruct					
	4N4O1	osyl-gl	481.211	481.213			
	2	ucose	4	0	0.85	POS	3.32
1428	C28H3	Physali	555.180	555.184			
	0O9	n B	8	0	7.43	NEG	5.76
		dendro					
1429	C21H3	monilis	483.183	483.183			
	2O11	ide b	5	6	4.76	POS	0.21
1430	C30H4	iridotec	487.341	487.341			
	6O5	toral a	4	6	11.47	POS	0.41
1431	C28H2	scirpusi	488.168	488.169			
	2O7	n A	8	6	3.83	POS	1.64
1432	C26H2	Corym	563.138	563.139			
	8O14	boside	4	5	4.17	NEG	1.95
		(6S,7E,9 R)-6,9-d ihydrox y-4,7-m egastig man-3- one-9- O- [α-L					
1433	C24H3	-arabin	563.232	563.233			
	8O12	opyran	7	6	4.35	NEG	1.60

		osyl-(1 →6)-(β- D-gluc opyran oside] 2-aceto xycaesa					
1434	C26H3	ldekari	490.243	490.243			
	2O8	n e	9	7	8.57	POS	-0.41
1435	C24H2	speciosi	491.152	491.154			
	8O12	de	6	0	5.21	POS	2.85
1436	C24H3	glansre	565.210	565.212			
	8O15	ginin B	6	2	4.31	NEG	2.83
		scroph					
1437	C24H2	uloside	492.180	492.183			
	6O10	A	2	3	3.35	POS	6.30
		20-hydr oxyecd ysone-					
1438	C30H4	2,3,acet	565.331	565.334			
	8O7	onide	0	6	6.29	NEG	6.37
		2α, 3α- dihydr oxy-urs -12-en-					
1439	C30H4	28-oic	493.330	493.329			
	6O4	acid	2	5	9.98	POS	-1.42
		Methyl hepta					
1440	C18H3	decano	567.534	567.534			
	6O2	ate	0	9	14.74	NEG	1.59

		Gentio					
		picrosi					
1441		de tetr					
	C24H2	aacetat	569.148	569.150			
	8O13	e	8	0	4.68	NEG	2.11
	C30H2	Blestria	498.188	498.190			
1442	4O6	rene B	9	0	5.76	POS	2.21
	C24H3	taxagifi	499.212	499.214			
1443	4O11	ne iii	0	7	5.18	POS	5.41
		Apigen					
		in 7-(6"					
		-p-cou					
1444		marylgl					
	C30H2	ucosid	577.133	577.134			
	6O12	e)	3	2	6.49	NEG	1.56
		vitexin-					
		2"-o-p-c					
1445	C30H2	oumara	577.133	577.134			
	6O12	te	1	1	6.68	NEG	1.73
		4',6"-di					
		acetyl					
1446	C25H2	puerari	503.148	503.151			
	6O11	n	6	7	5.30	POS	6.16
		iridoid					
1447	C26H3	glucosi	583.165	583.166			
	2O15	de	1	0	3.62	NEG	1.54
		Dihydr					
1448	C33H4	opseud	584.354	584.357			
	9NO5	oio	9	1	10.82	NEG	3.76
	C30H5	Theasa	507.366	507.367			
1449	0O6	pogeno	8	4	7.35	POS	1.18

		l A					
1450	C29H2	picrasi	508.206	508.202			
	2N4O4	dine n	3	1	2.24	POS	-8.26
		lycopos					
1451	C28H3	erramin	508.263	508.265			
	9NO6	e o	6	3	8.96	POS	3.34
		Limocit					
1452	C23H2	rin 3-gl	509.128	509.128			
	4O13	ucoside	1	6	5.09	POS	0.79
		Mulber					
1453	C34H2	rofuran	589.123	589.118			
	2O10	M	6	8	4.44	NEG	-8.15
		3-O-tra					
1454		ns-ferul					
	C27H2	oylquin	589.154	589.155			
	8O12	ic acid	4	3	4.54	NEG	1.53
1455	C30H3	Kushen	510.279	510.282			
	6O6	ol B	3	2	8.32	POS	5.49
1456	C30H5	Ganode	513.354	513.354			
	0O5	riol H	2	6	9.50	POS	0.78
		angeloy					
1457		lpodop					
	C27H2	hylloto	519.159	519.160			
	8O9	xin	3	9	3.73	POS	3.08
1458	C29H4	Sengost	519.296	519.296			
	4O9	erone	8	3	5.48	POS	-0.96
		4-O-β-					
1459		D-gluc					
		opyran					
	C26H3	osyloxy	603.151	603.150			
	2O14	benzoic	6	1	7.13	NEG	-2.49

		acid					
1460	C23H3	celepht	523.178	523.178			
	2O12	alide b	4	5	4.97	POS	0.19
1461	C36H3	isotrilo	611.234	611.233			
	6N2O5	bine	8	3	4.70	NEG	-2.45
		6''-o-p-c					
		oumaro					
1462	C29H3	ylaloesi	615.169	615.170			
	0O12	n	7	8	5.59	NEG	1.79
1463	C28H3	meliart	533.237	533.237			
	6O10	enin	3	7	8.53	POS	0.75
		Vitexin					
1464	C27H3	rhamn	623.159	623.160			
	0O14	oside	9	8	4.46	NEG	1.44
		5'-Meth					
1465	C32H2	oxybilo	627.124	627.119			
	2O11	betin	2	3	4.39	NEG	-7.81
		eriodict					
		yol-7,3-					
1466	C27H3	digluco	627.154	627.155			
	2O17	side	7	7	3.62	NEG	1.59
	C24H2						
1467	6N2O1	Prebeta	629.095	629.094			
	6S	nin	4	2	2.17	NEG	-1.91
1468	C30H2		543.127	543.127			
	2O10	gb1a	2	9	6.50	POS	1.29
		benzoyl					
1469	C30H3	isogomi	543.198	543.198			
	2O8	sin o	1	5	8.32	POS	0.74
1470	C29H3	Multifl	635.161	635.161			
	2O16	orin A	3	5	5.63	NEG	0.31

1471	(3S,8S,9 R,10R,1 3R,14S, 17R)-3- hydrox y-17-[(2 R,5R)-6 -hydro xy-6-m ethyl-5- [(2S,3R, 4S,5S,6 R)-3,4,5 -trihydr oxy-6- (hydro xymeth yl)oxan -2-yl]ox yhepta n-2-yl]- 4,4,9,13, 14-pent amethy l-1,2,3, 7,8,10,1 2,15,16, 17-deca hydroc yclopen ta[a]ph	635.414 8	635.415 6	12.57	NEG	1.26
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1472		enanthr					
		en-11-o					
		ne					
		12-benz					
		oxydap					
	C34H3	hnetoxi	637.179	637.182			
	4O10	n	6	1	0.96	NEG	3.92
		Lucidu					
1473	C27H3	moside	551.210	551.211			
	6O13	D	7	8	5.85	POS	2.00
		decum					
1474	C26H3	beside	553.188	553.190			
	2O13	D	6	1	5.52	POS	2.71
		methyl					
		(1S,4a					
		S,7aS)-7					
		-methyl					
		ene-1-					
		[(2S,3R,					
		4S,5S,6					
		R)-3,4,5					
1475		-trihydr					
		oxy-6-					
		[[(2R,3					
		R,4R,5					
		S,6R)-3,					
		4,5-trih					
		ydroxy-					
		6-meth					
	C23H3	yl-tetra	557.166	557.164			
	4O13	hydrop	7	9	5.21	POS	-3.23

		yran-2- yl]oxy methyl] tetrahy dropyr an-2-yl] oxy-4a, 5,6,7a-t etrahyd ro-1H-c yclopen ta[d]py ran-4-c arboxyl ate staphyl					
1476	C25H4	ionosid	557.257	557.256			
	2O12	e g	0	9	4.89	POS	-0.18
		neoharr					
1477	C30H3	ingtoni	558.206	558.208			
	3NO8	ne	2	0	3.85	POS	3.22
		2,3-did					
		ehydro-					
		2',7-dih					
		ydroxy-					
1478		4'-meth					
		oxy-3(2					
		',7-dihy					
		droxy-4					
	C32H2	'-metho	558.222	558.217			
	8O8	xyisofla	8	5	1.25	POS	-9.49

		van-5'- yl)flava n					
1479	C27H2		559.144	559.144			
	8O14	Maysin	0	6	5.15	POS	1.07
		6 , 6 '					
1480		-difeml					
	C28H3	oy}lisos	653.170	653.171			
	2O15	pinosin	9	6	4.43	NEG	1.07
1481	C27H3	Paeono	655.149	655.150			
	0O16	side	2	4	4.10	NEG	1.83
	C27H3						
1482	2N2O1	cadamb	567.186	567.190			
	0	ine	3	6	1.42	POS	7.58
1483	C28H3	Hordati	568.342	568.338			
	8N8O4	ne A	4	9	10.51	POS	-6.16
		Chryso phanol					
1484		8-(6-g alloylgl					
	C28H2	ucosid	569.128	569.128			
	4O13	e)	2	6	5.72	POS	0.70
1485	C35H6	gardner	659.473	659.473			
	6O8	ilin a	1	5	7.36	NEG	0.61
		Kaempferol 3- (2'',3''-d					
1486		iacetyl hamnos					
	C31H3	ide)-7-r	661.170	661.174			
	4O16	hamnos	8	1	6.02	NEG	4.99

		ide					
		butyl g					
1487	C34H5	anoder	573.384	573.381			
	2O7	ate A	8	7	15.17	POS	-5.41
1488	C34H3	orbiculi	665.235	665.229			
	6O11	n f	1	5	4.54	NEG	-8.42
		bijapon					
1489	C36H2	icaxant	667.156	667.151			
	8O13	hone	3	0	4.16	NEG	-7.94
1490	C36H3	Kwang	579.214	579.219			
	2N2O4	sine	0	7	5.80	POS	9.84
		5,6,4'-tr					
		ihydrox					
		yflavon					
		e 7-o- α					
		-1-2,3-di					
		-o-acety					
1491		lrhamn					
		opyran					
		osyl-(1					
		$\rightarrow$ 6)- β -					
		d-glucosyl					
	C31H3	pyra-no	677.165	677.168			
	4O17	side	5	9	5.21	NEG	5.02
		Secalon					
1492	C32H3	ic acid	683.159	683.160			
	0O14	A	7	7	4.47	NEG	1.46
		3 β -[(α -l					
		-arabin					
1493	C35H5	opyran	587.393	587.393			
	4O7	osyl)ox	6	9	7.78	POS	0.51

		y]-urs-1					
		2,19(29)					
		-dien-2					
		8-oicaci					
		d					
		18-Deh					
		ydroures					
		olic aci					
1494		d 3-ara					
	C35H5	binosid	587.394	587.394			
	4O7	e	2	2	7.11	POS	0.00
	C33H5	aspidos	685.344	685.344			
1495	2O12	ide a	1	1	6.67	NEG	0.00
		5'-hydr					
		oxyiso-					
		muron					
1496		ulatol-2					
		'5'-di-O					
	C29H3	-glucosi	687.213	687.213			
	8O16	de	0	6	4.52	NEG	0.87
	C38H3	glycobi	695.185	695.182			
1497	2N2O9	smine f	0	6	6.21	NEG	-3.45
		isobeta					
		nidin-6-					
		o-rham					
1498	C30H3	nosyl s					
	6N2O1	ophoro	695.181	695.188			
	7	side	9	0	1.01	NEG	8.77
		rhodeas					
1499	C33H5	apogen	595.383	595.383			
	4O9	in-3-o-β	4	7	9.03	POS	0.50

1500		-d-glucopyranoside 5-ene-methyl-7,12-didehydr oxy-cho late-3-o - α -l-rhamnopyranosyl -(1 $\rightarrow$ 4)- β -d-glucurono-					
	C37H5	pyrano	709.375	709.378			
1501	8O13	side	7	1	8.04	NEG	3.38
	C24H4	Isolychnose	711.219	711.219			
1502	2O21	nose	4	7	1.27	NEG	0.42
	C38H4	orthosiphol a	721.277	721.282			
1503	4O11	Ginger glycolipid A	4	0	4.60	NEG	6.38
	C33H5	Prodelphinidin	721.365	721.365			
1504	6O14	Prodelphinidin B	2	2	10.00	NEG	0.00
	C30H2	kaempferol-3-o	611.137	611.138			
1505	6O14	kaempferol-3-o	3	4	5.21	POS	1.80
	C39H3	-(2'',6''-di-o-(e)	739.177	739.172			
	2O15		5	2	4.18	NEG	-7.17

		-p-cou maroyl- β-d-glu copyra noside)					
1506	C31H4 2O10	Asclepi n	613.241 0	613.241 0			
					7.63	POS	0.00
1507	C33H5 0O9	cimilact one a	613.334 1	613.334 4			
					7.33	POS	0.49
1508	C32H4 0O17	phellosi de	741.223 1	741.223 9			
					4.66	NEG	1.08
		osmant					
1509	C29H3 6O13	huside B6	615.208 4	615.206 6			
					5.21	POS	-2.93
		1,3,6-tri hydrox y-2-met hylanth raquino ne-3-O- (3'-O-ac etyl)-α- rhamno syl(1→					
1510	C28H3 0O16	2)-gluc oside	623.159 2	623.159 9			
					5.22	POS	1.12
		Kaempf erol--4 , 7-di					
1511	C29H3 4O15	methyl ether	623.195 6	623.196 3			
					5.84	POS	1.12

		compla					
1512	C28H3	natusid	625.176	625.176			
	2O16	e	0	2	4.43	POS	0.16
		taxuspi					
1513	C31H3	nanane	625.203	625.204			
	8O11	d	6	1	8.30	POS	0.80
1514	C39H6	Smilani	769.438	769.438			
	4O12	ppin A	3	1	10.77	NEG	-0.13
		2,3,4,7,-					
		tetrame					
		thoxyx					
		anthon					
		e-1-o-b					
1515		eta-d-x					
		ylopyra					
		nosyl-					
		(1-6)-be					
		ta-d-gl					
	C28H3	ucopyr	627.192	627.192			
	4O16	anoside	0	0	4.99	POS	0.00
		3',5-dih					
		ydroxy-					
		4'-meth					
		oxyflav					
1516		one 7-o					
		-α- rha					
		mnoses					
		yl(1.6)-					
	C28H3	β-d-glu	628.222	628.222			
	4O15	coside	0	8	5.21	POS	1.27
1517	C37H3	Simula	636.270	636.270	1.41	POS	-0.16

	4N2O7	noquin	7	5			
		oline					
		Viscum					
1518	C29H3	neoside	637.176	637.176			
	2O16	IV	7	5	5.64	POS	-0.31
1519	C29H3	yadanz	643.222	643.223			
	8O16	ioside I	9	1	4.48	POS	0.31
		Narirut					
1520	C33H4	in 4'-gl	787.229	787.229			
	2O19	ucoside	0	6	4.66	NEG	0.76
1521	C36H5	abrusos	647.378	647.378			
	4O10	ide A	8	9	7.89	POS	0.15
		Spinasa					
1522	C42H6	ponin	793.437	793.437			
	6O14	A	4	7	9.75	NEG	0.38
1523	C30H3	matteu	656.253	656.254			
	8O15	cinin	7	3	5.21	POS	0.91
		(25r)-sa					
		mogeni					
		n 3-o-β					
		-d-gluc					
1524		opyran					
		osyl(1					
		→2)-β-					
		d-galac					
	C39H6	topyran	801.427	801.427			
	4O14	oside	2	5	7.57	NEG	0.37
		licorice					
1525	C42H6	saponin	805.399	805.400			
	2O15	e c2	4	5	9.05	NEG	1.37
1526	C35H4	kaempf	809.213	809.214	4.11	NEG	0.49

	0O19	erol-3-o	8	2			
		-lysima					
		chiatrio					
		side					
1527	C32H3	Ikarisos	680.254	680.254			
	8O15	ide B	1	5	4.61	POS	0.59
		Hexand					
1528	C39H5	raside	821.286	821.286			
	0O19	D	4	9	5.05	NEG	0.61
		apiogly					
1529	C41H6	cyrrhizi	823.410	823.411			
	2O14	n	4	3	8.81	NEG	1.09
		(2S)-2-					
		(1-hydr					
		oxy-1-					
		methyl-					
		ethyl)-9					
		-(2S,3					
		R,4R,5					
		S,6R)-3,					
		4,5-trih					
1530		ydroxy-					
		6-meth					
		ylol-tet					
		rahydr					
		opyran-					
		2-yl]ox					
		y-2,3-di					
		hydrof					
	C20H2	uro[3,2-	847.265	847.266			
	4O10	g]chro	8	2	4.64	NEG	0.47

1531		men-7-one glycoside k(p					
	C40H6	eriploc	847.429	847.431			
	6O16	ae)	1	2	7.86	NEG	2.48
1532		glaucogenin c3-o-β-d-cymaropyranosyl-(1→4)-α-l-diginopyranosyl-(1→4)-β-d-thevetopyranoside 7-o-(4-β-d-glucopyranosyloxy-3-methoxy-benzoyl)secologanolica cid staminolacton					
	C42H6	vetopyr	853.416	853.419			
	4O15	anoside	5	6	9.99	NEG	3.63
1533							
	C30H4	anolica	711.215	711.213			
	0O18	cid	7	2	6.08	POS	-3.52
1534	C38H4	stamin	713.255	713.256			
	2O12	olacton	8	3	7.53	POS	0.70

		es B					
		luteolifl					
		avan-(4					
		beta->					
1535		8)-eriod					
		ictyol-5					
	C36H3	-glucisi	723.198	723.195			
	4O16	de	2	1	0.84	POS	-4.29
1536	C33H4	Arillani	725.230	725.229			
	0O18	n A	2	5	6.62	POS	-0.97
	C41H8	SM(d1					
1537	1N2O6	8:1/18:	729.587	729.589			
	P	1)	7	1	12.81	POS	1.92
		Macrop					
1538	C40H4	hyllosi	875.223	875.224			
	4O22	de A	4	3	5.02	NEG	1.03
	C35H3						
1539	8N8O6	pariphy	737.214	737.220			
	S	llin b	1	4	8.27	POS	8.55
		Acaceti					
		n 7-(2G					
1540		-rhamn					
		osyl)-ru					
	C34H4	tinosid	739.242	739.243			
	2O18	e	8	6	5.21	POS	1.08
		deacylb					
1541	C39H6	rownio	739.426	739.426			
	2O13	side	3	3	5.17	POS	0.00
1542	C39H6	Torvosi	741.441	741.441			
	4O13	de C	8	9	6.59	POS	0.13
1543	C37H4	(3R,6R,	742.353	742.353	7.25	POS	0.13

	9N7O8	9R,12S, 15R,21 S)-3,9-b is(benz yl)-15-i sobutyl -6-meth yl-12-m ethylol- 1,4,7,10, 13,16,19 -heptaz abicycl o[19.3. 0]tetrac osane- 2,5,8,11, 14,17,20 -hepton e acetylas	3	4			
1544	C47H7	tragalo	909.484	909.485			
	4O17	side	6	0	9.93	NEG	0.44
		26-o-β- d-glucosyl(25r, s)-5α-furostan					
1545	C45H7	e-12-on	915.459	915.459			
	2O19	e-20(22)	5	5	5.53	NEG	0.00

		-en-3β, 26-diol- 3-o-β-d -glucop yranos yl-(1→ 4)-β-d- galacto pyrano side (5beta,2 5S)-Spir ostan-3 beta,15 alpha,2 3alpha- diol-3- O-D-gl ucopyr anosyl- (1-2)-be ta-D-ga lactopy					
1546	C39H6	ranosid	757.436	757.436			
	4O14	e	5	7	5.78	POS	0.26
		gitogen in 3-O- β-D-gal					
1547	C39H6	actopyr	758.469	758.468			
	4O13	anoside	3	9	9.63	POS	-0.53
1548	C44H5	ervadiv	759.376	759.382	7.28	POS	7.90

	6N4O5	aricatin	2	2			
		e a					
1549	C45H7	Tubero	947.484	947.485			
	4O18	side E	7	2	9.12	NEG	0.53
1550	C46H7	wattosi	947.484	947.485			
	6O20	de c	7	2	10.17	NEG	0.53
		phyllae					
1551	C33H4	mblicin	767.224	767.230			
	4O19	B	9	9	9.61	POS	7.82
		macrost					
1552	C45H7	emonos	979.474	979.475			
	4O20	ide g	5	0	4.91	NEG	0.51
		26-o-β-					
		d-glucosyl-(25					
		s)-3β,5					
		β,6α,22					
		ξ,26-pentahydroxyl-5					
1553		β-furostane 3-o					
		-α-l-rhamnopyranosyl					
		-(1→4)-β-d-glucopyranosyl					
	C45H7	copyranoside	981.490	981.490			
	6O20	noside	2	7	4.94	NEG	0.51
1554	C42H6	(4aS,6aS)	787.464	787.462	9.52	POS	-2.79

8O12	R,6aS,6	7	5
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bR,8aR,
 9R,10S,
 12aR,14
 bS)-10-
 [(2R,3
 R,4S,5S,
 6S)-4,5-
 dihydr
 oxy-6-
 methyl-
 3-[(2S,
 3R,4R,5
 R,6S)-3,
 4,5-trih
 ydroxy-
 6-meth
 yl-2-tet
 rahydr
 opyran
 yl]oxy]-
 2-tetrah
 ydropy
 ranyl]o
 xy]-9-(h
 ydroxy
 methyl)
 -2,2,6a,
 6b,9,12
 a-hexa
 methyl-

1555		1,3,4,5, 6,6a,7,8, 8a,10,1 1,12, 3,4-dih ydroxy phenyl ethanol -8-o-[4- o-trans- caffeoyl -β-d-ap iofuran osyl(1 →3)]-β- d-glucop -pyrano syl-(1→ 6)]-β-d- glucop					
	C34H4	yransio	795.230	795.231			
1556	4O20	de	6	2	4.80	POS	0.75
	C42H7	ginseno	805.475	805.473			
	0O13	side La	7	3	9.04	POS	-2.98
1557		Heliant					
	C53H8	hoside	1093.55	1093.54			
1558	6O21	A	03	29	6.45	NEG	-6.77
		Acetylj					
1559	C54H8	ujubosi	1131.55	1131.55			
	6O22	de B	50	72	8.58	NEG	1.86
	C50H6	tenuifol	1161.35	1161.35	5.06	NEG	-3.19

1560	6O31	iose m	90	53			
	C54H8	celosin	1161.52	1161.53			
	4O24	G	88	11	6.45	NEG	1.98
1561		panicul					
	C54H6	atonoid	1255.33	1255.34			
	6O31	a	69	70	5.20	NEG	8.05
1562	C57H7	tenuifol	1265.37	1265.37			
	0O32	iose k	29	53	5.22	NEG	1.90
		sophor					
1563	C59H9	aflavosi	1281.60	1281.60			
	6O27	de	75	98	7.13	NEG	1.79
	C44H7		873.484	873.484			
1564	2O17	as-1 a	3	3	7.31	POS	0.00
		26-o-be					
		ta-d-gl					
1565		ucopyr					
		anosyl-					
		3beta,2					
		6-dihyd					
		roxy-5-					
		cholesle					
		n-16,22-					
		dioxo-3					
		-o-alph					
		a-l-rha					
		mnopy					
		rano-sy					
		l-(1-2)-b					
		eta-d-gl					
	C45H7	ucopyr	901.479	901.479			
	2O18	anoside	1	1	5.27	POS	0.00

1566	C45H7	terrestr	904.531	904.528			
	4O17	osin b	0	7	9.54	POS	-2.54
		macrost					
1567	C45H7	emonos	936.516	936.516			
	4O19	ide l	2	2	5.76	POS	0.00
		Sandos					
1568	C48H7	aponin	957.507	957.506			
	6O19	A	0	2	8.31	POS	-0.84
		licorice					
1569	C48H7	saponin	985.461	985.462			
	2O21	a3	9	9	6.34	POS	1.01
		Trigofo					
1570	C51H8	enoside	1049.55	1049.55			
	4O22	E1	25	26	6.47	POS	0.10
		Trigofo					
1571	C51H8	enoside	1065.54	1065.54			
	4O23	F	64	70	6.06	POS	0.56
		Trigofo					
1572	C56H9	enoside	1197.58	1197.58			
	2O27	G	72	85	5.44	POS	1.09
		Solanig					
1573	C56H9	roside	1213.58	1213.58			
	2O28	F	14	31	5.01	POS	1.40
1574	C64H1	platyco	1423.66	1423.64			
	04O33	side i	15	84	5.32	POS	-9.20
